Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

Synthesis of honeycomb-like Cu-based metal-organic framework and its carbon dioxide adsorption behaviour

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S1 Crystallographic Data of $Cu_2(dhtp)(CH_3OH)_{2.73}(DMF)_{0.25}(H_2O)_{1.33}$

S2 TGA/DTG analyses in presence of different co-solvents

S3 N_2 Adsorption/desorption isotherms in presence of different co-solvents

S4 SEM images for the different $Cu_2(dhtp)$ materiales synthesized

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S1 Crystallographic Data of $Cu_2(dhtp)(CH_3OH)_{2.73}(DMF)_{0.25}(H_2O)_{1.33}$

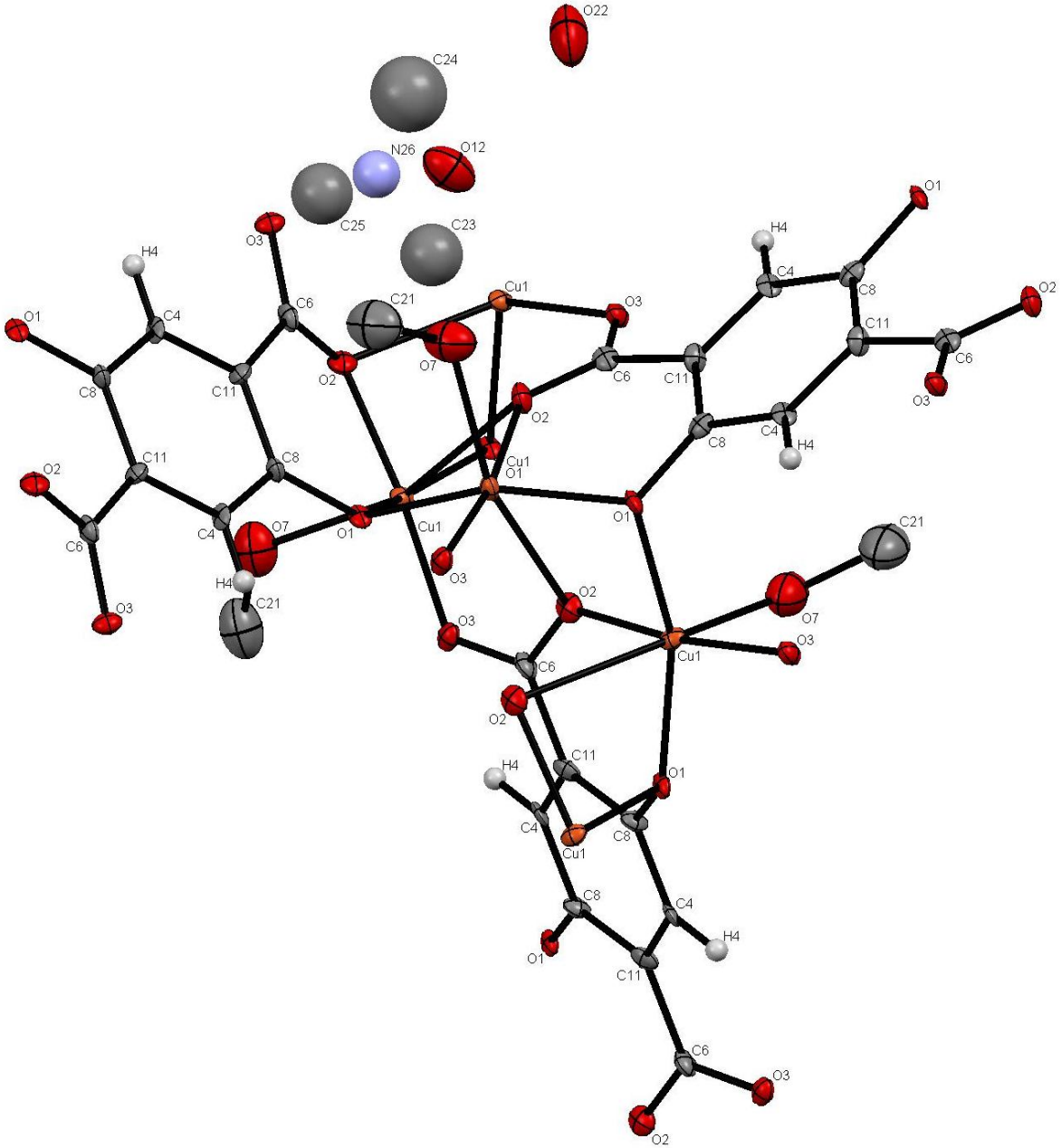

Table S1. Crystal data and structure refinement for compound $Cu_2(dhtp)(CH_3OH)_{2.73}(DMF)_{0.25}(H_2O)_{1.33}$

Identification code	$Cu_2(dhtp)$
Empirical formula	C11.17 H18.02 Cu2 N0.25 O10
Moiety Formula	C8H2O6Cu2, 2.4 MeOH, 0.25 DMF, 1.333 H2O
Moiety Formula Including Squeeze Results	C8H2O6Cu2, 2.73 MeOH, 0.25 DMF, 1.333 H2O
Formula weight	426.71
Temperature	100(2) K
Wavelength	1.54178 A
Crystal system, space group	Trigonal, R-3
Unit cell dimensions	a = 25.9972(11) A alpha = 90 deg. b = 25.9972(11) A beta = 90 deg. c = 6.2587(3) A gamma = 120 deg.
Volume	3663.3(3) A^3
Z, Calculated density	9, 1.741 Mg/m^3
Absorption coefficient	3.692 mm^-1
F(000)	1879
Crystal size	0.20 x 0.02 x 0.02 mm
Theta range for data collection	5.90 to 65.34 deg.
Limiting indices	-30<=h<=29, -29<=k<=22, -5<=l<=7
Reflections collected / unique	3601 / 1332 [R(int) = 0.0668]
Completeness to theta = 65.34	94.5 %
Max. and min. transmission	0.9298 and 0.5255
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1332 / 4 / 125
Goodness-of-fit on F^2	0.994

Final R indices [I>2sigma(I)]	R1 = 0.0454, wR2 = 0.1107
R indices (all data)	R1 = 0.0689, wR2 = 0.1198
Largest diff. peak and hole	0.561 and -0.472 e.A^-3

S2 TGA/DTG analyses in presence of different co-solvents

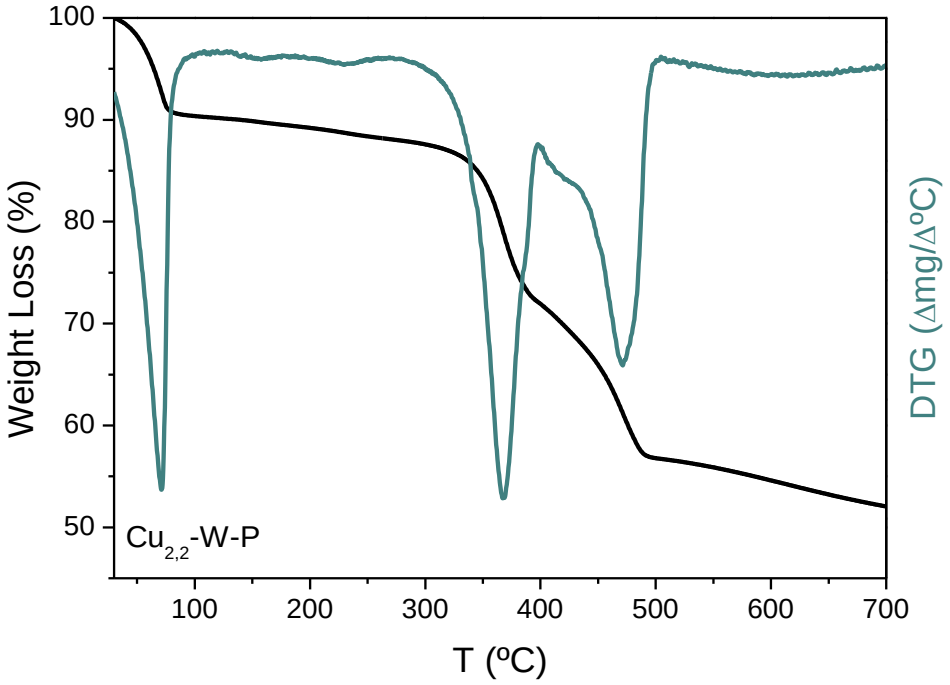

Fig. S1 TGA/DTG of the sample $Cu_{2.2}$-W-P.

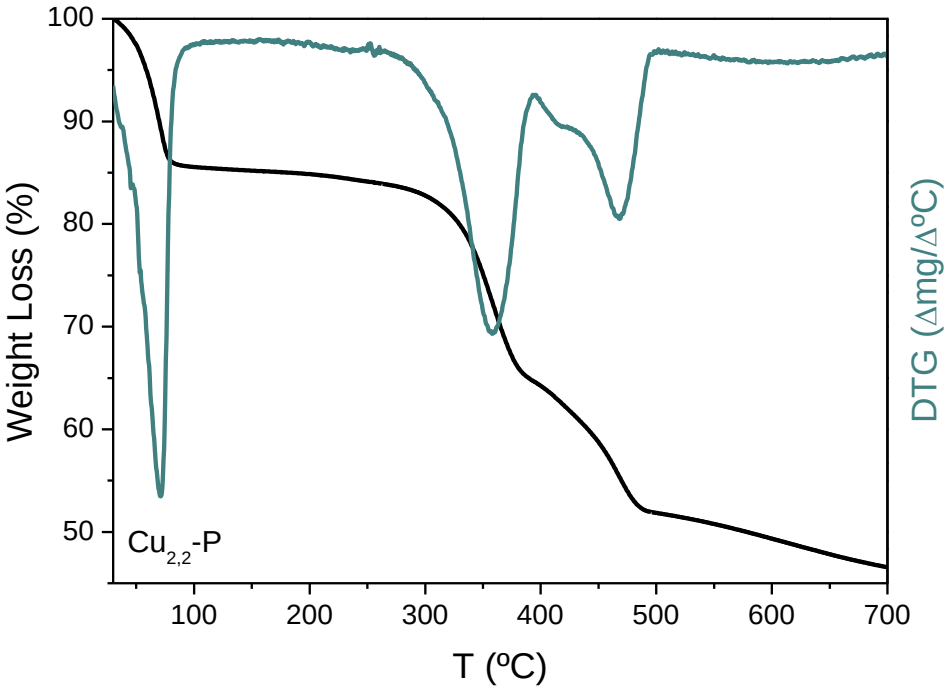

Fig. S2 TGA/DTG of the sample $Cu_{2.2}$-P.

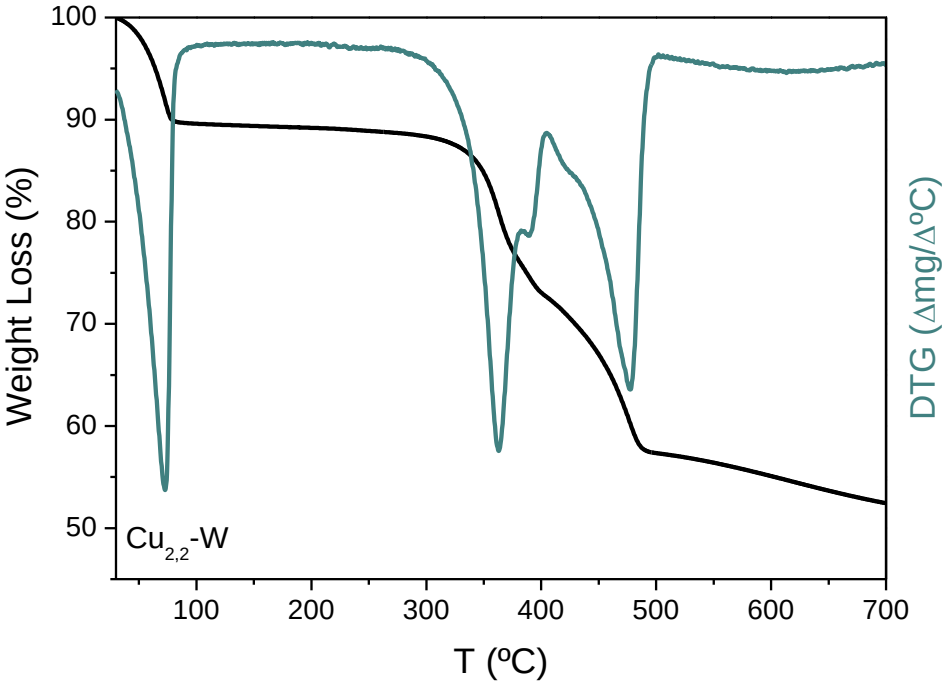

Fig. S3 TGA/DTG of the sample $Cu_{2.2}$-W.

S3 N_2 Adsorption/desorption isotherms in presence of different co-solvents

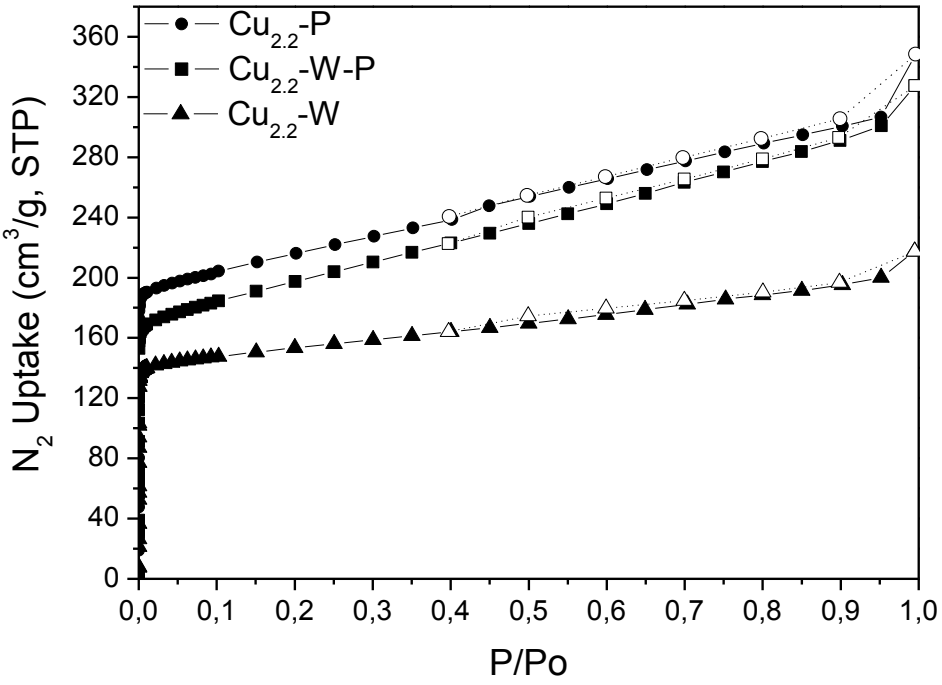

Fig. S4 N_2 isotherms at 77 for the samples synthesized with different co-solvents

S4 SEM images for the different Cu_2(dhtp) materiales synthesized

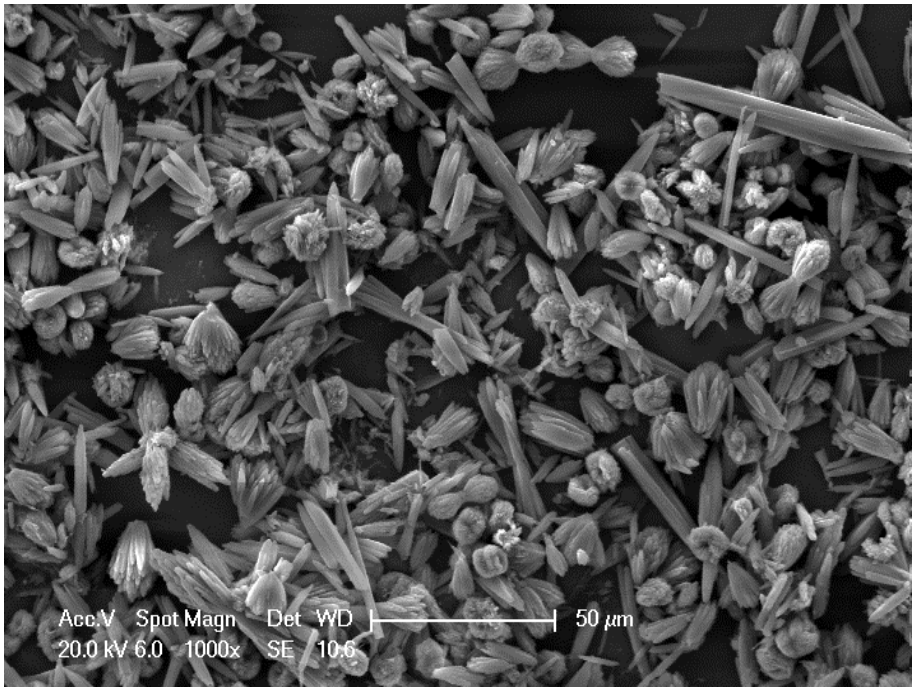

Fig. S5 SEM micrograph of the sample $Cu_{2.2}$-W-P. The scale of the micrograph corresponds to 50 µm

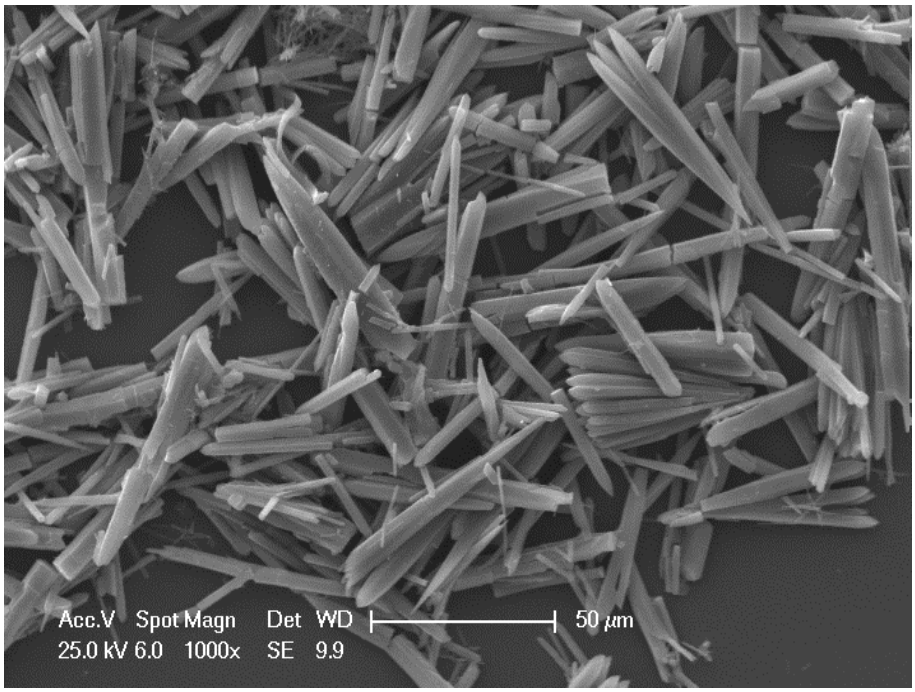

Fig. S6 SEM micrograph of the sample $Cu_{2.2}$-P. The scale of the micrograph corresponds to 50 µm

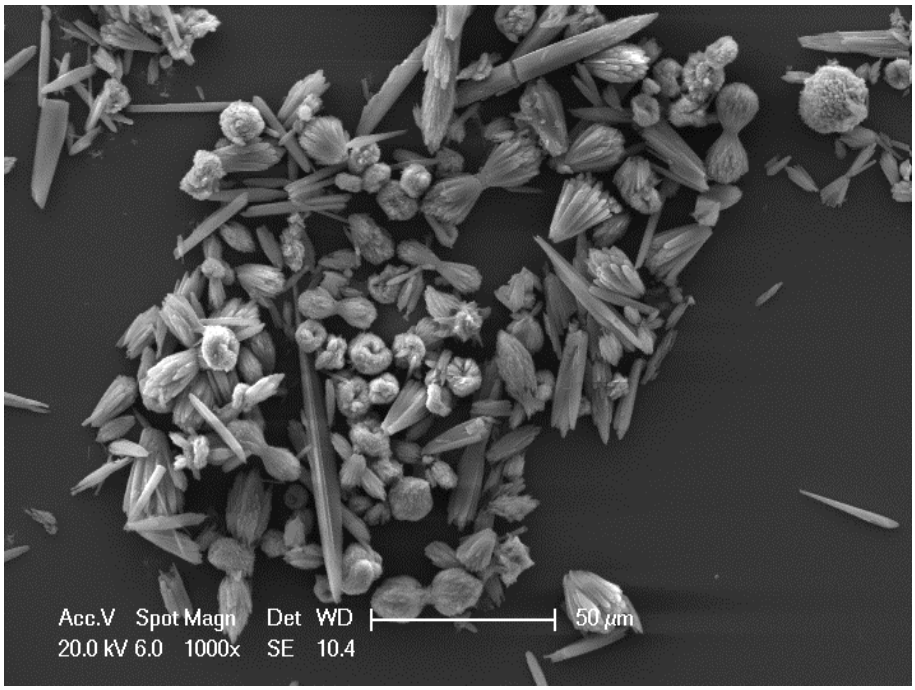

Fig. S7 SEM micrograph of the sample $Cu_{2.2}$-W. The scale of the micrograph corresponds to 50 µm