Copper-organic frameworks assembled from *in-situ* generated 5-(4-pyridyl)tetrazole building blocks: synthesis, structural features, topological analysis and catalytic oxidation of alcohols

Supplementary information

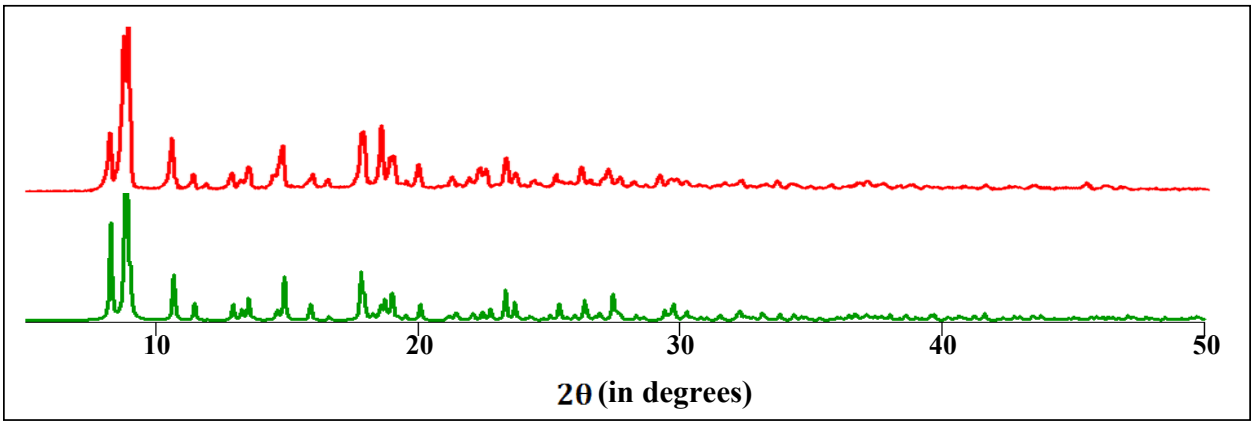

Fig. S1: PXRD patterns of the compound **1**: simulated (green) and bulk sample (red)

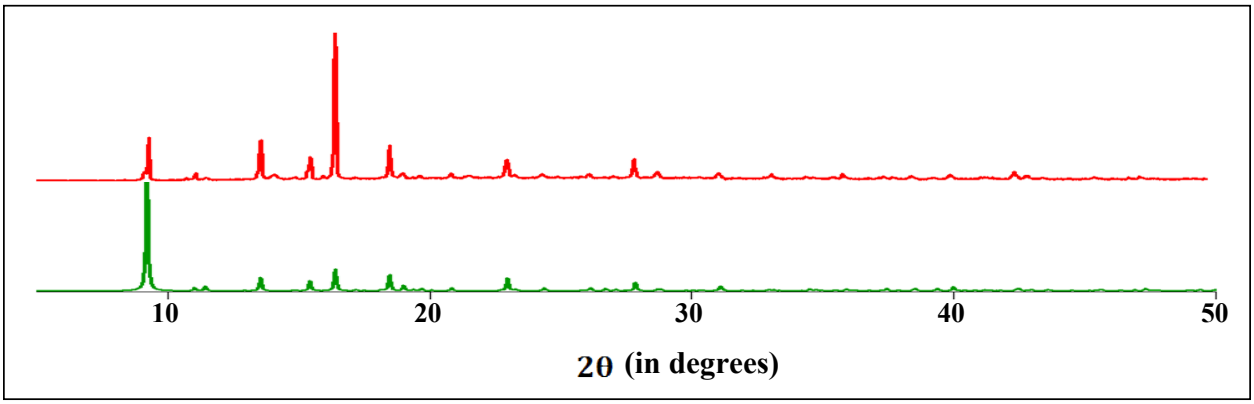

Fig. S2: PXRD patterns of the compound **2**: simulated (green) and bulk sample (red)

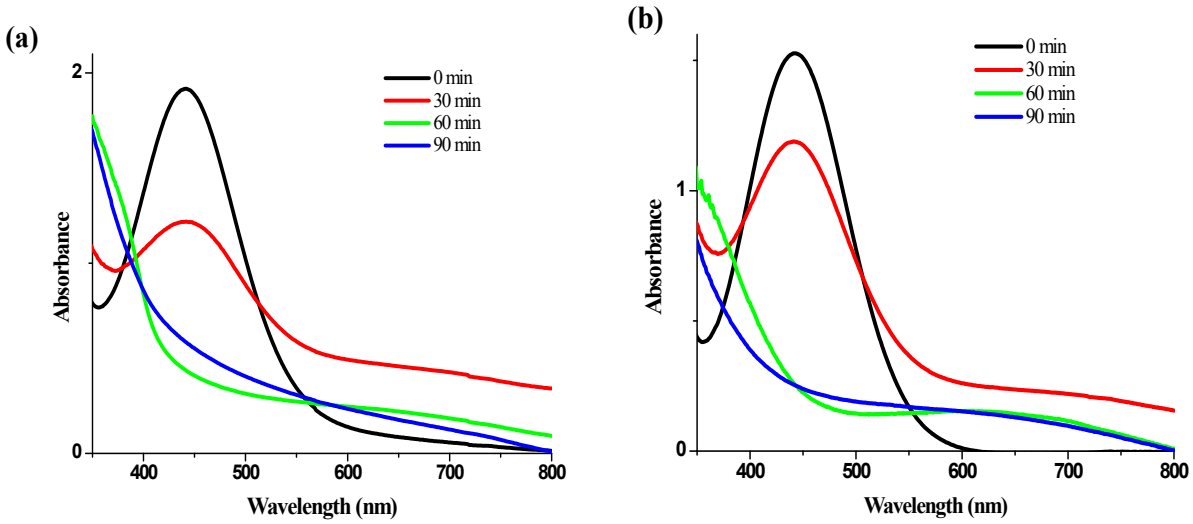

Fig S3: UV-vis spectra recorded while monitoring solvent-free oxidation of cyclohexanol by TBHP/TEMPO system in the presence of **1** (a) and **2** (b).

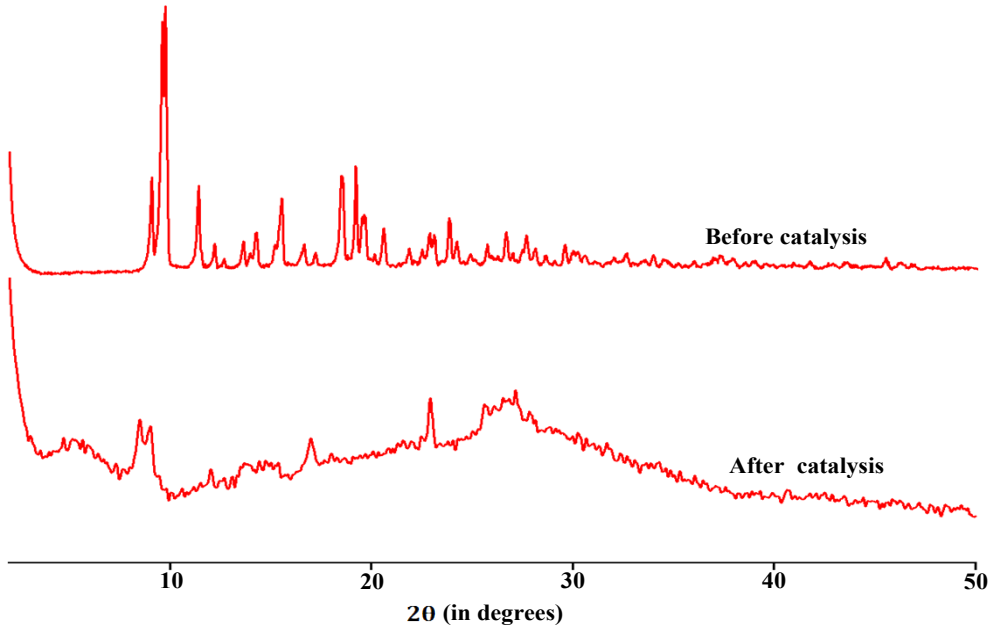

Fig. S4: Comparison of PXRD patterns of the compound **1** before and after using as catalyst.

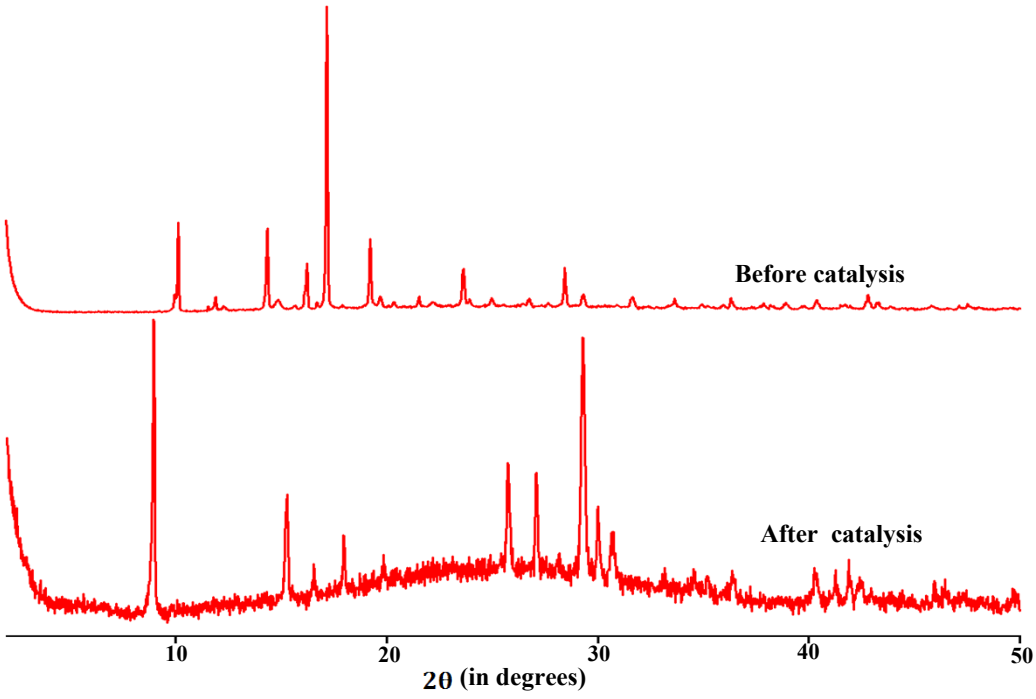

Fig. S5: Comparison of PXRD patterns of the compound **2** before and after using as catalyst.

Table S1. MW-assisted oxidation of secondary alcohols by TBHP with **1** and **2** as catalyst precursors.[a]

Entry	Catalyst Precursor	Substrate	TOF[b] (h^{-1})	Yield[c] (%)
1			397	79
2[d]			350	70
3[e]			185	37
4[f]		1-phenylethanol	15	3
5[g]			10	2
6[h]			460	92
7[i]			130	78
8[j]			110	22
9[k]			400	80
10			290	58
11[d]			265	53
12[e]			145	29
13[f]		cyclohexanol	10	2
14[g]			20	4
15[h]			335	67
16[i]			92	55
17[j]			75	15
18[k]			285	57
19	**1**		315	63
20[e]			105	21
21[h]		2-hexanol	385	77
22[j]			115	23
23[k]			315	63
24			285	57
25[e]		3-hexanol	95	19
26[h]			370	74
27			190	38
28[e]			60	12
29[h]		2-octanol	270	54
30[j]			85	17
31[k]			200	40
32			235	47
33[e]		3-octanol	85	17
34[h]			315	63
35			430	86
36[d]			405	81
37[e]			205	41
38[f]		1-phenylethanol	25	5
39[g]			15	3
40[h]			495	99

41[i]			142	85
42[j]			165	33
43[k]			425	85
44			210	42
45[d]			195	39
46[e]			140	28
47[f]		cyclohexanol	10	2
48[g]			15	3
49[h]			320	64
50[i]			67	40
51[j]			95	19
52[k]	**2**		209	42
53			335	67
54[e]		2-hexanol	155	31
55[h]			405	81
56			330	66
57[e]			110	22
58[h]		3-hexanol	420	84
59[j]			80	16
60[k]			335	67
61			290	58
62[e]		2-octanol	90	18
63[h]			395	79
64			255	51
65[e]			70	14
66[h]		3-octanol	335	67
67[j]			60	12
68[k]			245	49
69			35	7
70[e]		1-phenylethanol	15	3
71[h]			55	11
72	$CuCl_2$[l]	cyclohexanol	10	2
73		2-hexanol	30	6
74		3-hexanol	20	4
75		2-octanol	30	6
76		3-octanol	15	3

[a] Reaction conditions unless stated otherwise: 5 mmol of substrate, 10 μmol (0.2 mol% *vs*. substrate) of catalyst precursor, 10 mmol of TBHP (70% aq.), 80 ºC, 1 h reaction time, microwave irradiation (10 W). [b] Turnover frequency = number of moles of product per mol of catalyst per hour (turnover number per hour). [c] Moles of ketone product per mol of alcohol. [d] 20 mmol of TBHP (4 eq.). [e] H_2O_2 (10 mmol) 30% aqueous solution instead of TBHP. [f] In the presence of Ph_2NH (5 mmol). [g] In the presence of $CBrCl_3$ (5 mmol). [h] In the presence of TEMPO (5 mol% *vs*. substrate). [i] 3 h reaction time. [j] T = 50 ºC. [k] T = 100 ºC. [l] Included for comparative purposes.