Electronic Supplementary Information

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Water-soluble Al(III), Fe(III) and Cu(II) formazanates: synthesis, structure, applications in alkane and alcohol oxidations

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1. Catalysis

Table S1. MW-assisted oxidation of cyclohexane to cyclohexanol and cyclohexanone catalyzed by formazanate metal complexes **1-3**[a].

Entry	Cat.	Cat. (μmol)	CyH (mmol)	Yield (%)[b]			TON[c]
				K	A	Total	
1	**2**	0.50	1.0	3.5	19.5	23.0	230
2		0.50	2.5	1.4	8.4	9.8	490
5		1.00	0.5	8.4	7.5	15.9	79
6		1.00	1.0	2.0	26.6	28.6	286
7		1.00	1.5	1.7	27.2	28.9	433
8		1.00	2.0	1.9	22.6	24.5	490
9		1.00	2.5	2.9	8.3	11.2	279
10		1.50	1.0	9.6	18.9	28.4	189
11		1.50	2.5	5.1	10.7	15.8	263
12		1.75	1.0	6.1	17.9	24.0	120
13		1.75	2.5	4.9	10.3	15.2	224
14		2.00	1.0	6.2	14.3	20.5	117
15		2.00	2.5	4.0	5.8	9.8	123
16	**3**	0.50	1.0	2.8	15.8	18.6	372
17		0.50	2.5	2.2	5.8	8.0	400
18		1.00	0.5	7.9	7.9	15.8	79
19		1.00	1.0	3.8	16.6	20.4	204
20		1.00	1.5	1.6	15.1	16.7	251
21		1.00	1.75	1.3	12.1	13.4	235
22		1.00	2.0	1.0	11.0	12.0	240
23		1.00	2.5	0.5	9.2	9.7	242
24		1.50	1.0	5.0	12.1	17.1	116
25		1.50	2.5	1.8	9.4	11.2	164
26		2.00	1.0	1.4	13.2	14.6	73
27		2.00	2.5	1.8	8.1	9.9	123

[a] Reaction conditions unless stated otherwise: 3 mL MeCN, farmazan catalyst (0.5-2.0 μmol), cyclohexane (1.0-2.5 mmol), oxidant, H_2O_2 (5 mmol), 80 ºC, 20 W, 1 h. [b] Moles of product/100 moles of cyclohexane (A = cyclohexanol and K = cyclohexanone). [c] Overall TON (moles of products/mole of catalyst). GC analysis performed upon addition of PPh_3 (conversion of CyOOH into cyclohexanol prior to GC analysis).

2. X-ray analysis

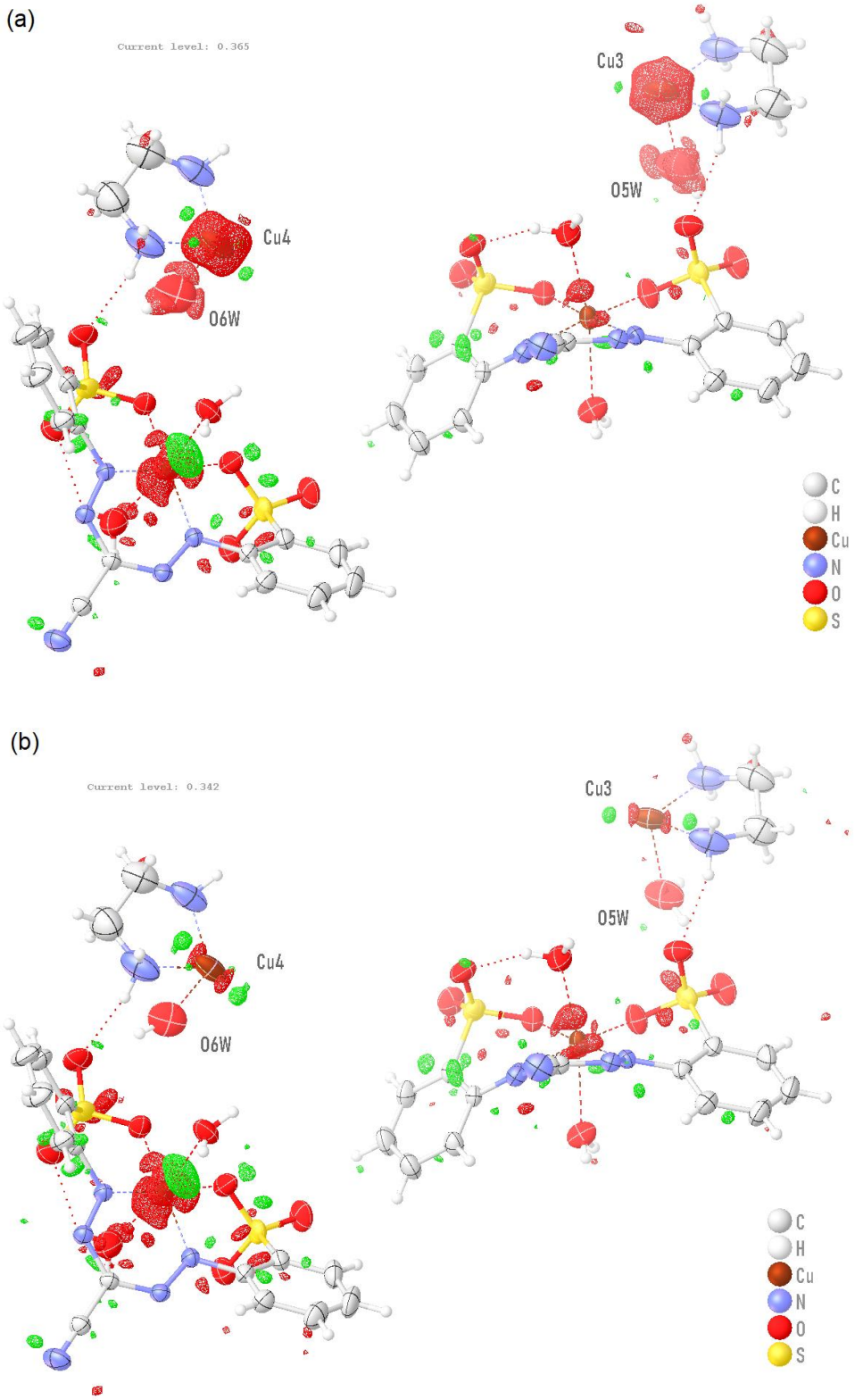

Figure S1. Residual density maps before (a) and after (b) freely refinement of occupancies of Cu3, Cu4 and of the attached water molecules O5w, O6w.