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Supporting Information

Copper-amidocarboxylate Based Metal Organic Macrocycle and Framework: Synthesis, Structure and Catalytic Activities towards Microwave assisted Alcohol Oxidation and Knoevenagel reaction

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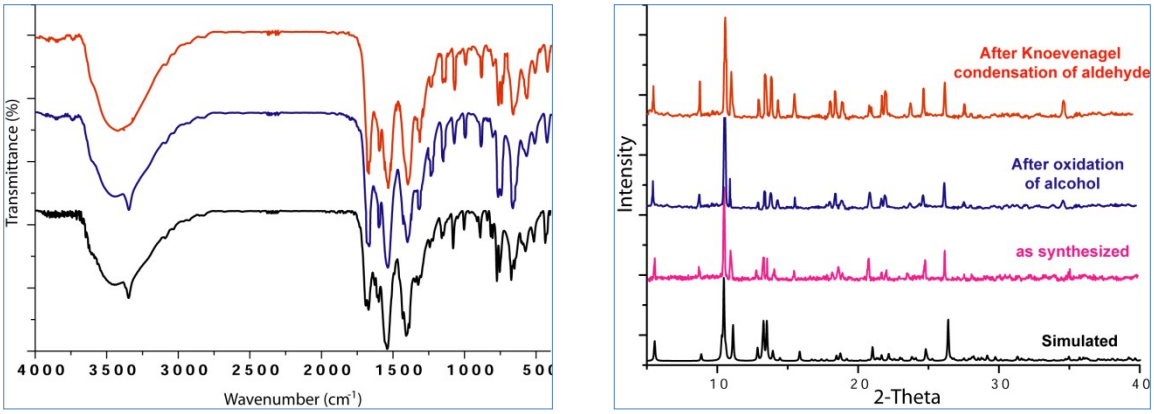
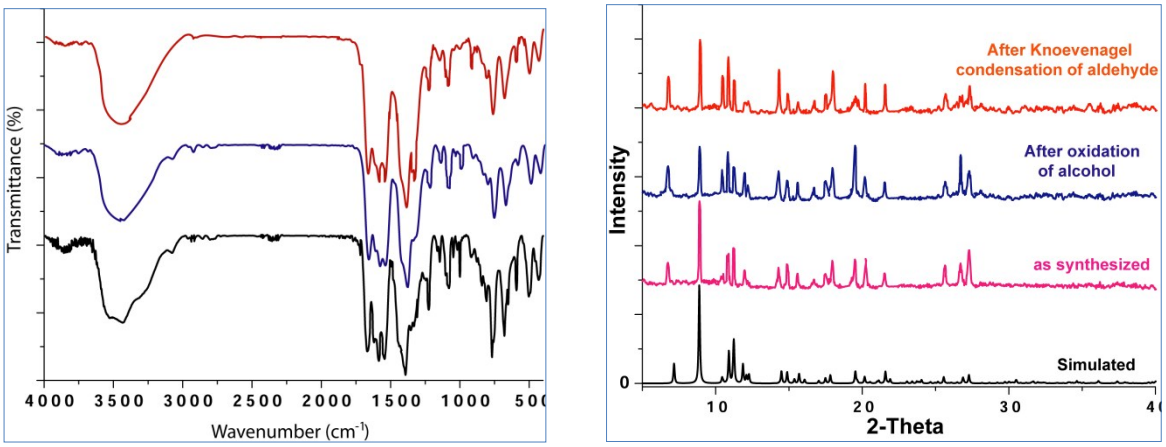


A B

Figure S1 A) FT-IR spectra of **1** before (in black), after oxidation of alcohol (in blue) and Knoevenagel condensation of aldehyde (in red). B) Powder XRD diffractograms of **1** simulated (in black), as synthesized (in pink) and after catalytic oxidation of alcohol (in blue) and Knoevenagel condensation of aldehyde (in red).



A B

Figure S2 A) FT-IR spectra of **2** before (in black), after oxidation of alcohol (in blue) and Knoevenagel condensation of aldehyde (in red). B) Powder XRD diffractograms of **2** simulated (in black), as synthesized (in pink) and after catalytic oxidation of alcohol (in blue) and Knoevenagel condensation of aldehyde (in red).

Table S1: Crystal data and structure refinement details		
	1	**2**
Formulae	$C_{49}H_{51}Cu_4N_9O_{25}$	$C_{27}H_{27}CuN_5O_8$
Mol. wt.	1420.15	613.07
Crystal system	Triclinic	Monoclinic
Space group	P-1	$P2_1/n$
Temperature /K	296	296
Wavelength /Å	0.71073	0.71073
a /Å	8.8368(5)	9.1236(8)
b /Å	9.9857(6)	15.7177(14)
c /Å	16.3956(9)	19.9209(17)
α/°	91.165(2)	90
β/°	103.967(2)	93.270(2)
γ/°	92.411(2)	90
V/ $Å^3$	1402.06(14)	2852.0(4)
Z	1	4
Density/Mgm^{-3}	1.682	1.428
Abs. Coeff. /mm^{-1}	1.591	0.823
F(000)	724	1268
Refl. collected	30829	45098
Refl. unique	5744	5202
Max. 2θ/°	26.426	25.382
Complete to 2θ (%)	99.6	99.8
Refl. with I > 2σ(I)	4556	3161
Data/Restraints/Parameters	5744/131/404	5202/18/334
Goof (F^2)	1.037	1.001
R1 [I > 2s(I)]	0.0466	0.0541
wR2 [I > 2s(I)]	0.1195	0.1104
R1 [all data]	0.0621	0.1089
wR2 [all data]	0.1304	0.1314

Table S2: Selected bond distances (Å) and angles (°) for compounds **1**-**2**

1	Cu1-O2, 1.911(2); Cu1-O6, 1.927(2); Cu1-O7, 1.967(3); Cu1-O7, 2.000(3); Cu1-O9, 2.428(4); Cu1-Cu1', 2.9391(8); Cu2-O5, 1.920(3); Cu2-O1, 1.934(2); Cu2-O7, 1.957(3); Cu2-O8, 1.975(3); Cu2-O10A, 2.375(9); O1-Cu2, 1.934(2); O1-Cu2A, 1.940(5); O7-Cu2A, 1.775(5); O7-Cu1, 2.000(3); O8-Cu2A, 2.406(6); O5-Cu2A, 2.019(5) <O2-Cu1-O6, 86.65(10); <O2-Cu1-O7, 177.45(10); <O6-Cu1-O7, 95.73(11) ; <O2-Cu1-O7, 93.60(11); <O6-Cu1-O7, 163.77(13); <O7-Cu1-O7', 84.39(12); <O2-Cu1-O9, 92.88(14); <O6-Cu1-O9, 94.57(15); <O7-Cu1-O9, 86.00(14); <O7-Cu1-O9, 101.63(14); <O2-Cu1-Cu1', 135.33(8); <O6-Cu1-Cu1', 136.07(8); <O7-Cu1-Cu1', 42.63(8); <O7-Cu1-Cu1', 41.76(7); <O9-Cu1-Cu1', 95.19(10); <Cu2A-Cu2-O5, 87.9(4); <Cu2A-Cu2-O1, 80.1(4); <O5-Cu2-O1, 158.77(14); <Cu2A-Cu2-O7, 64.7(4); <O5-Cu2-O7 ,95.87(11); <O1-Cu2-O7, 94.76(10); <Cu2A-Cu2-O8, 120.5(4); <O5-Cu2-O8, 83.67(12); <O1-Cu2-O8, 87.40(11); <O7-Cu2-O8, 174.66(15); <Cu2A-Cu2-O10A, 144.8(7); <O5-Cu2-O10A, 91.0(3); <O1-Cu2-O10A, 108.9(3); <O7-Cu2-O10A, 80.4(5); <O8-Cu2-O10A, 94.3(5); <Cu2A-O7-Cu1, 128.4(2); <Cu2-O7-Cu1, 117.73(13); <Cu2A-O7-Cu1, 123.9(2); <Cu2-O7-Cu1, 114.02(14); <Cu1-O7-Cu1, 95.61(12); <Cu2-Cu2A-O7, 94.5(5); <Cu2-Cu2A-O1, 79.1(5); <O7-Cu2A-O1, 100.7(2); <Cu2-Cu2A-O5, 71.9(4); <O7-Cu2A-O5, 98.5(2); <O1-Cu2A-O5, 146.2(3); <Cu2-Cu2A-O8, 45.0(4); <O7-Cu2A-O8, 139.5(3); <O1-Cu2A-O8, 76.0(2); <O5-Cu2A-O8, 71.31(18); <Cu2-Cu2A-H7O, 120.4(8); <O7-Cu2A-H7O, 26.9(7); <O1-Cu2A-H7O, 110.5(11); <O5-Cu2A-H7O, 99.1(11); <O8-Cu2A-H7O, 163.9(8);
2	Cu1-O1, 1.949(3); Cu1-O5, 1.953(3); Cu1-O2, 1.959(3); Cu1-O6, 1.970(3); Cu1-O7, 2.142(3); Cu1-Cu1', 2.6246(10). <O1-Cu1-O5, 87.98(14); <O1-Cu1-O2, 168.82(13); <O5-Cu1-O2, 89.30(13); <O1-Cu1-O6, 91.00(14); <O5-Cu1-O6, 168.69(12); <O2-Cu1-O6, 89.54(13); <O1-Cu1-O7, 94.51(14); <O5-Cu1-O7 93.89(13); <O2-Cu1-O7, 96.50(14); <O6-Cu1-O7, 97.42(12); <O1-Cu1-Cu1', 84.14(10; <O5-Cu1-Cu1', 82.80(9); <O2-Cu1-Cu1', 84.75(9); <O6-Cu1-Cu1', 85.89(9); <O7-Cu1-Cu1', 176.46(10).

Table S3: Hydrogen bond geometry (Å, °) in compounds 1-2

Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D–H···A(°)
1	O12-H12O···O4	0.82	1.95	2.766(3)	179.7
	N1-H1N···O12	0.70(4)	2.36(4)	3.004(4)	154(5)
	N1-H1N···N2	0.70(4)	2.31(4)	2.639(4)	110(4)
	N3-H3N···N2	0.75(4)	2.18(4)	2.614(4)	118(4)
	O8-H8O···N4	0.866(19)	2.70(3)	3.481(6)	151(4)
	O8-H8O···O11	0.866(19)	2.30(3)	3.064(8)	147(4)
	O8-H8O···O10A	0.866(19)	2.57(4)	3.201(13)	130(4)
	O8-H8O···O10B	0.866(19)	2.17(4)	2.93(2)	146(4)
	O7-H7O···O9	0.928(19)	2.45(3)	3.016(5)	119(3)
	C7-H7···O12	0.93	2.64	3.252(4)	124
	C5-H5···O3	0.93	2.42	2.977(4)	118
	C20-H20···O4	0.93	2.41	2.981(4)	119
	C22-H01E···O10A	0.96	2.52	3.064(9)	116
	C22-H01E···O10B	0.96	2.81	3.170(2)	103
	C22-H01F···O10B	0.96	2.58	3.150(3)	118
2	N3-H3N···O3	1.06(9)	2.47(9)	3.290(5)	133(6)
	N1 H1N N2	0.95(9)	2.23(9)	2.713(6)	111(7)
	C5-H5···O3	0.93	2.29	2.833(7)	116.8
	C24-H24A···O4	0.96	2.65	3.483(10)	145.5