

Electronic Supplementary Material

Mononuclear Copper(II) Complexes of Arylhydrazone of 1*H*-Indene-1,3(2*H*)-dione as Catalysts for the Oxidation of 1-Phenylethanol in Ionic Liquid Medium

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1. X-ray analyses

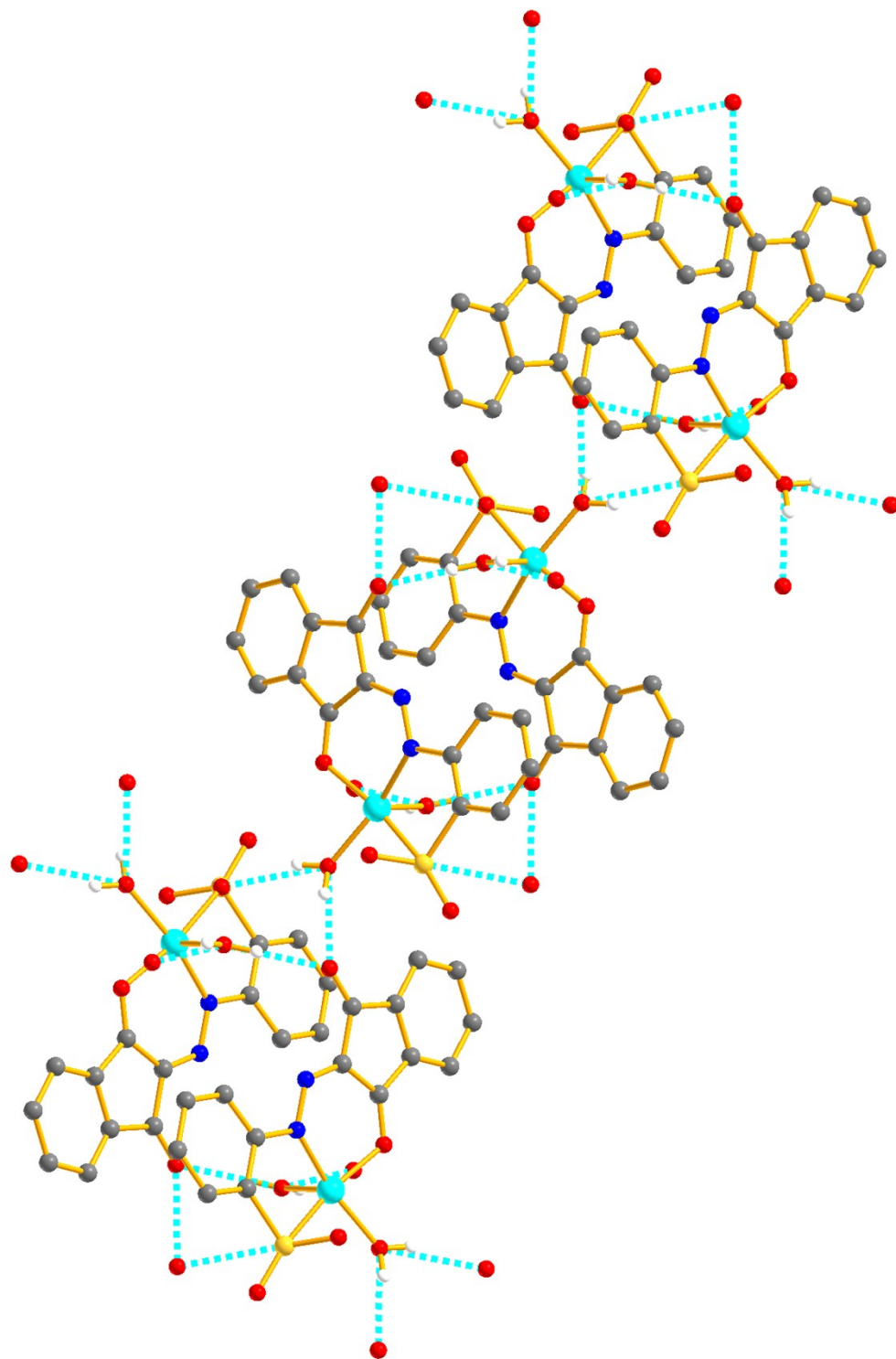
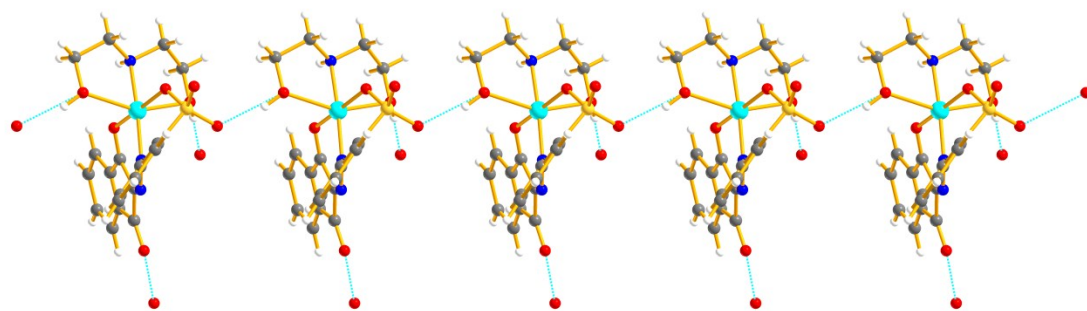
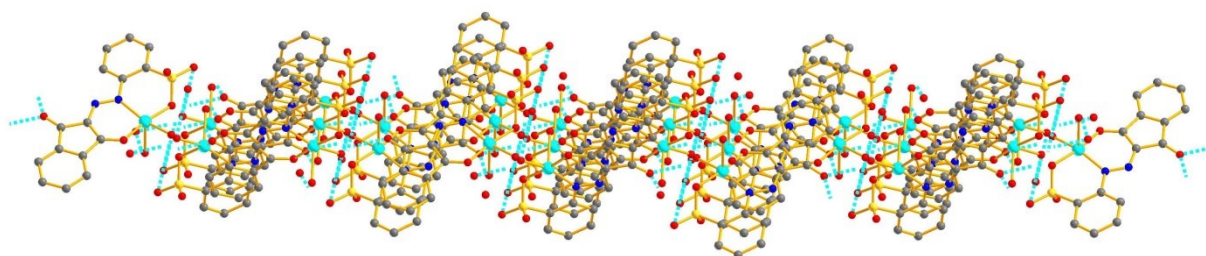


Figure S1 – Fragment of the infinite 2D network (along *b* and *c*) found in **1**. H-atoms not involved in these interactions are omitted for clarity.

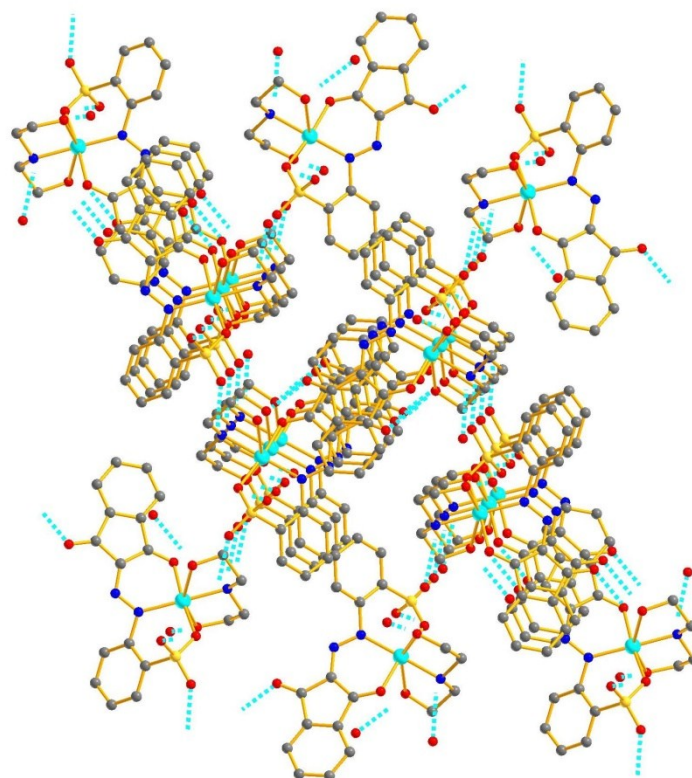


B

Figure S2 – Fragment of the infinite 1D (along *a*) chain found in **2**.



A



B

Figure S3 – Fragments of the 3D networks found in **1** (A) and **2** (B).

Table S1. Crystallographic data and structure refinement details for **1** and **2**.

	1	2
Empirical formula	C ₁₅ H ₁₄ CuN ₂ O ₈ S	C ₁₉ H ₁₈ CuN ₃ O ₇ S
fw	445.88	495.96
Temperature (K)	296(2)	296(2)
Cryst. Syst.	Monoclinic	Monoclinic
Space group	<i>P</i> 21/ <i>c</i>	<i>P</i> 21/ <i>n</i>
<i>a</i> (Å)	8.9126(7)	7.4989(3)
<i>b</i> (Å)	10.0253(7)	19.3512(6)
<i>c</i> (Å)	18.9226(16)	13.6935(5)
β , °	90.499(3)	94.3580(10)
<i>V</i> (Å ³)	1690.7(2)	1981.36(12)
<i>Z</i>	4	4
ρ_{calc} (g cm ⁻³)	1.752	1.663
μ (Mo K α) (mm ⁻¹)	1.465	1.257
<i>F</i> (000)	908	1016
Rfl. total/unique/obs	21696/3035/2288	20735/3644/3063
R _{int}	0.0789	0.0340
GOOF	1.054	1.097
R1 ^a (<i>I</i> ≥ 2 σ)	0.0491	0.0432
wR2 ^b (<i>I</i> ≥ 2 σ)	0.1246	0.1066

^a $RI = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. ^b $wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table S2. Selected bond distances (Å) and angles (°) for **1** and **2**.

1		2	
C6 N1	1.451(5)	C1 N2	1.335(4)
C7 N2	1.338(5)	C2 O1	1.247(4)
C8 O2	1.222(5)	C9 O2	1.222(4)
C15 O1	1.250(5)	C10 N1	1.428(4)
N1 N2	1.291(4)	C17 N3	1.462(5)
N1 Cu1	2.017(3)	C18 O6	1.429(5)
O1 Cu1	1.935(3)	C19 N3	1.499(5)
O3 Cu1	1.967(3)	C20 O7	1.434(5)
O4 Cu1	2.214(4)	N1 N2	1.296(3)
O11 Cu1	1.958(3)	N1 Cu1	1.993(2)
O1 Cu1 O11	170.21(12)	N3 Cu1	2.013(3)
O1 Cu1 O3	83.16(13)	O1 Cu1	1.960(2)
O11 Cu1 O3	87.17(13)	O5 Cu1	1.980(2)
O1 Cu1 N1	95.67(12)	O6 Cu1	2.509(3)
O11 Cu1 N1	93.99(12)	O7 Cu1	2.374(3)
O3 Cu1 N1	161.69(16)	O1 Cu1 O5	172.01(10)
O1 Cu1 O4	89.32(15)	O1 Cu1 N1	91.73(10)
O11 Cu1 O4	90.32(15)	O5 Cu1 N1	93.73(10)
O3 Cu1 O4	96.77(17)	O1 Cu1 N3	86.06(10)
N1 Cu1 O4	101.49(15)	O5 Cu1 N3	88.75(11)
		N1 Cu1 N3	176.45(11)
		O1 Cu1 O7	94.09(11)
		O5 Cu1 O7	90.77(11)
		N1 Cu1 O7	99.47(10)
		N3 Cu1 O7	77.95(11)