

Electronic Supplementary Information

for

Sulfonated Schiff Base Copper(II) Complexes as Efficient and Selective Catalysts in Alcohol Oxidation: Syntheses and Crystal Structures

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Table S1. Crystallographic Data for **1 – 5**.

	1	2	3	4	5
Formula	C ₁₄ H ₁₉ NO ₈ S	C ₁₄ H ₁₅ CuNO ₇ S	C ₂₇ H ₂₈ CuN ₄ O ₇ S	C ₃₈ H ₃₂ Cu ₂ N ₄ O ₁₀ S ₂	C ₃₂ H ₃₈ Cu ₂ N ₂ O ₁₄ S ₂
FW	361.36	404.87	616.13	895.92	865.84
Crystal colour	Yellow	Brown	Green	Green	Green
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	P21/c	P 21/c	P-1	P21/n	P21/n
<i>a</i> /Å	6.9329(10)	8.599(5)	7.9237(2)	8.149(2)	7.7522(10)
<i>b</i> /Å	12.2785(18)	14.399(5)	11.2344(4)	16.476(5)	17.119(2)
<i>c</i> /Å	19.091(3)	12.598(5)	16.0644(5)	13.478(4)	13.2121(14)
α /°	90	90.00	103.893(1)	90	90.00
β /°	98.079(5)	96.196(5)	96.378(2)	94.476(10)	92.839(4)
γ /°	90	90.00	94.347(1)	90	90.00
<i>V</i> /Å ³	1609.0(4)	1550.7(12)	1371.79(7)	1804.1(9)	1751.2(4)
<i>Z</i>	4	4	2	2	2
2 θ /°	5.44–51.40	4.764– 51.414	5.102– 52.382	4.944– 50.668	4.758– 52.864
μ (Mo K α)/mm ⁻¹	0.245	1.581	0.925	1.362	1.406
ρ_{calcd} /g cm ⁻³	1.492	1.734	1.492	1.649	1.642
<i>F</i> (000)	760	828	638	916	892
Index ranges	–8< <i>h</i> <8	–10< <i>h</i> <10	–9< <i>h</i> <9	–9< <i>h</i> <9	–9< <i>h</i> <9
	–14< <i>k</i> <14	–17< <i>k</i> <17	–13< <i>k</i> <13	–19< <i>k</i> <19	–21< <i>k</i> <21
	–23< <i>l</i> <23	–15< <i>l</i> <15	–19< <i>l</i> <19	–16< <i>l</i> <16	–16< <i>l</i> <16
Reflections collected	18998	17681	23731	25898	30546
Independent reflections	3053	2964	5473	3260	3592
<i>R</i> _{int}	0.1429	0.0631	0.0341	0.0899	0.0282
<i>R</i> ₁ ^a / w <i>R</i> ₂ ^b [<i>I</i> > 2 σ (<i>I</i>)]	0.0576/0.0924	0.0439/0.0966	0.0414/0.1034	0.0432/0.0807	0.0321/0.0796
<i>R</i> ₁ ^a / w <i>R</i> ₂ ^b [for all <i>F</i> _o ²]	0.1272/0.1102	0.0686/0.1049	0.0563/0.1125	0.0731/0.0886	0.0357/0.0816
GOF on <i>F</i> ²	1.065	1.031	1.074	1.033	1.040

Table S2. Hydrogen bond geometry [$\text{\AA}$, $^\circ$] in **1** – **5**.

Compound	D–H $\cdots$ A	D $\cdots$ A	H $\cdots$ A	D–H $\cdots$ A
1	N1–H1N $\cdots$ O1	2.745	2.130	127.10
	N1–H1N $\cdots$ O3	2.918	2.268	131.31
	O1–H1 $\cdots$ O6	2.760	1.761	166.18
	O6–H6OA $\cdots$ O5'	3.047	2.177	163.43
	O6–H6OB $\cdots$ O7'	2.715	1.831	161.44
	O7–H7OA $\cdots$ O8	2.699	1.812	165.20
	O7–H7OB $\cdots$ O5'	2.986	2.064	176.32
	O8–H8OA $\cdots$ O4'	2.772	1.870	177.17
	O8–H7OA $\cdots$ O6'	3.019	2.157	161.78
2	O3–H30A $\cdots$ O1'	2.826	1.934	161.69
	O3–H30B $\cdots$ O4'	2.666	1.714	177.88
	O4–H40A $\cdots$ O2'	3.041	2.458	122.81
	O4–H40B $\cdots$ O6'	2.769	1.854	171.83
3	O7–H1A $\cdots$ O5'	2.895	2.094	167.75
	O7–H1B $\cdots$ O4'	2.847	2.045	166.28
4	C18–H18 $\cdots$ O4'	3.292	2.366	173.32
5	O6–H6E $\cdots$ O7	2.654	1.786	176.46
	O7–H7WA $\cdots$ O4	2.791	1.977	161.15
	O7–H7WB $\cdots$ O2	2.940	2.110	171.89

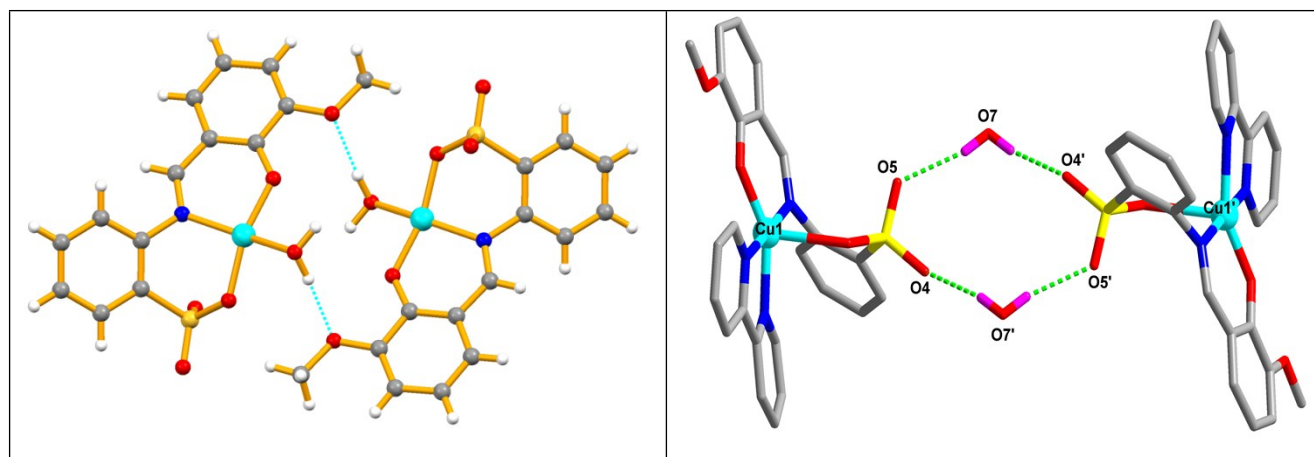


Figure S1. The $R_2^2(14)$ and $R_4^4(12)$ graph sets found in **2** and **3**.

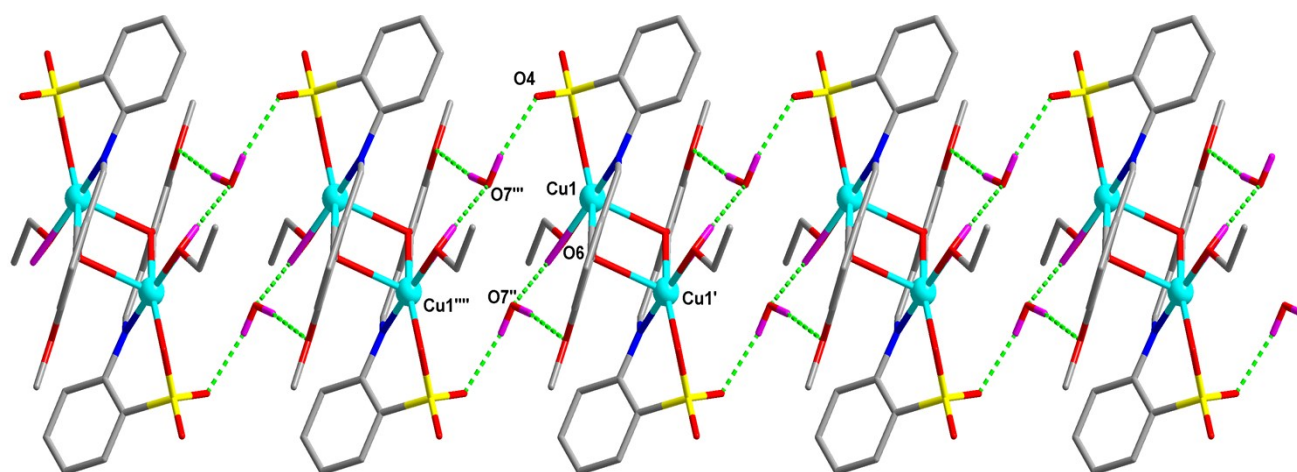


Figure S2. Presentation of the H-bond supported 1D chain in **5**.