Electronic Supplementary Information

Mononuclear copper(II) complex immobilized in mesoporous silica: efficient heterogeneous catalyst for aerobic oxidation of benzylic alcohols

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Table S1 Metrical parameters for H-bonding, C–H···π, π···π interactions in compound **1**

	D–H···A	D–H distance (Å)	H···A distance (Å)	D···A distance (Å)	D–H···A angle (deg)	symmetry code
H–bonding	N(1)–H(1)···O(6)	0.86	2.00	2.793(3)	153.00	1+x,y,z
	N(2)–H(2)···O(1)	0.86	1.89	2.602(3)	139.00	
	N(3)–H(3A)···O(3)	0.86	2.00	2.792(3)	153.00	-1+x,y,z
	N(4)–H(4)···O(4)	0.86	1.88	2.601(3)	140.00	
	C–H···π[a] atoms		H···π distance (Å)	C···π distance (Å)	C–H···π distance (Å)	symmetry code
C–H···π	C(33)–H(33)···πC(23)···C(28)[b]		3.02	3.75	135	1-x,½+y,1-z; 1-x,-½+y,1-z
	C(13)–H(13)···πC(37)···C(42)[c]		2.91	3.67	138	
	C(32)–H(32)···πC(16)···H(21)[c]		2.80	3.61	144	
	π···π[a] atoms			π···π, distance (Å)		symmetry code
π···π	πC(2)···C(7)···πC(23)···C(28)			3.53		1+x,y, z; -1+x,y,z

^{1}H NMR spectrum of the ligand HL

The ^{1}H NMR spectrum of the ligand HL has been recorded in $CDCl_3$ and their chemical shift values with their spectral assignments are given in the Experimental Section. Scheme S1 shows the proton labelling for the ligand HL. HL exhibits (Fig. S1) a low-field resonance at 14.02 ppm due to the hydrogen bonded O-H···N proton (H1). The singlet at 9.37 is due to the proton attached to the amide nitrogen, H2. The aromatic proton, H3 is observed as singlet. It may be noted that H4 is observed as doublet while H5 and H6 are observed as triplet. The methyl proton H7 appears at 2.30 ppm as a singlet. Fig.S1 shows the ^{1}H NMR spectrum of the ligand HL.

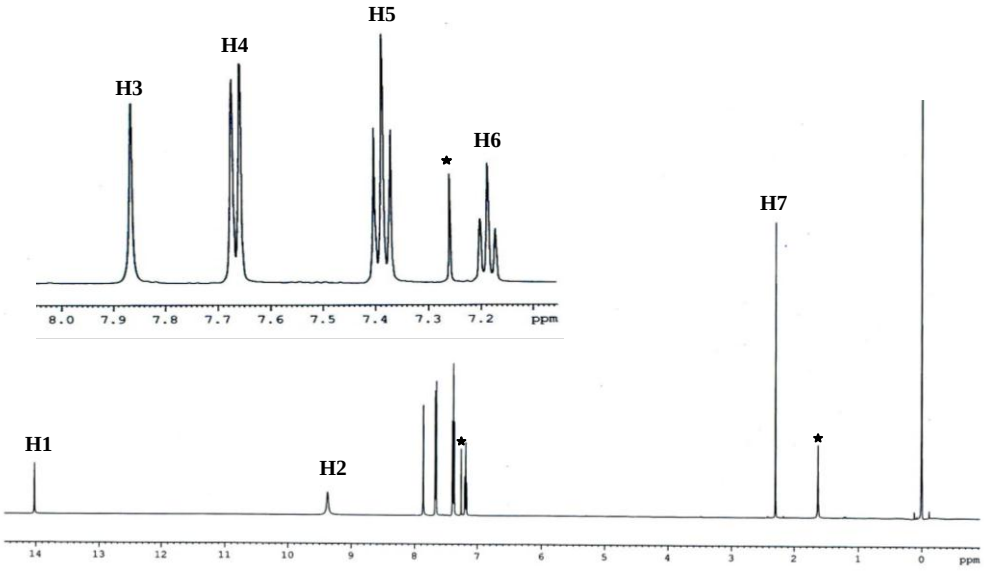
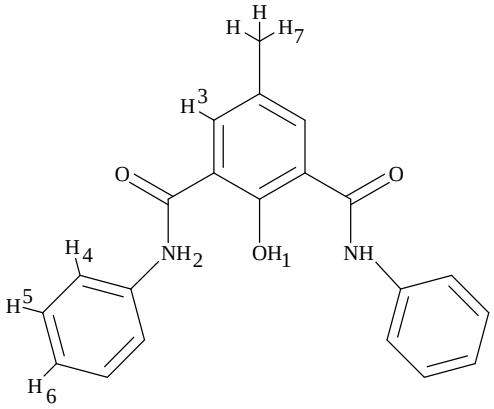


Fig. S1 ^{1}H NMR spectrum of the ligand (HL) in $CDCl_3$. Inset shows the aromatic region. The solvent peaks are marked with asterisks.



Scheme S1 Proton labelling scheme for ligand HL

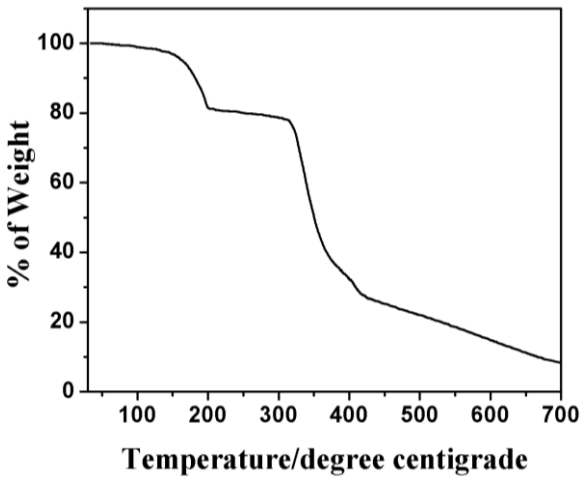


Fig. S2 TGA Curve of complex1 in N_2 atmosphere.

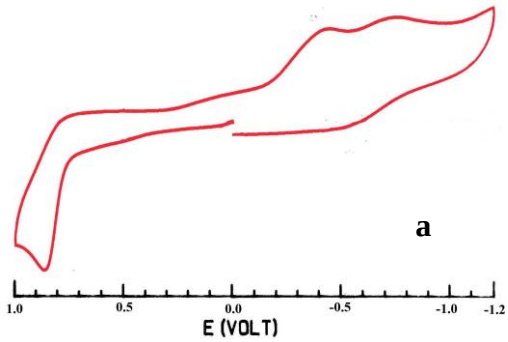


Fig. S3a Cyclic voltammogram of the complex **1** in DMF.

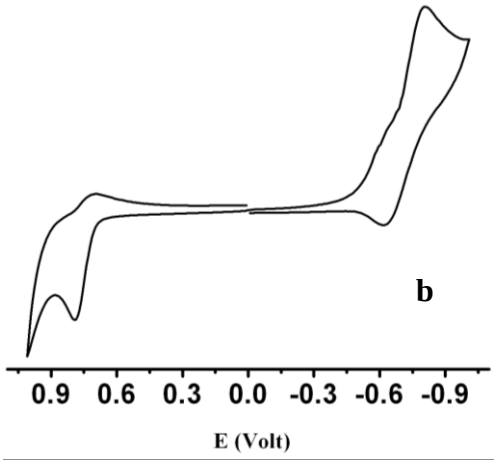


Fig. S3b Cyclic voltammogram of the ligand HL in DMF.

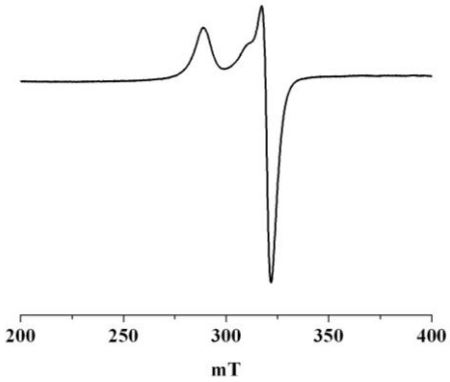


Fig. S4 X-band EPR spectrum of complex **1** in a frozen DMF solvent at liquid N_2 temperature.

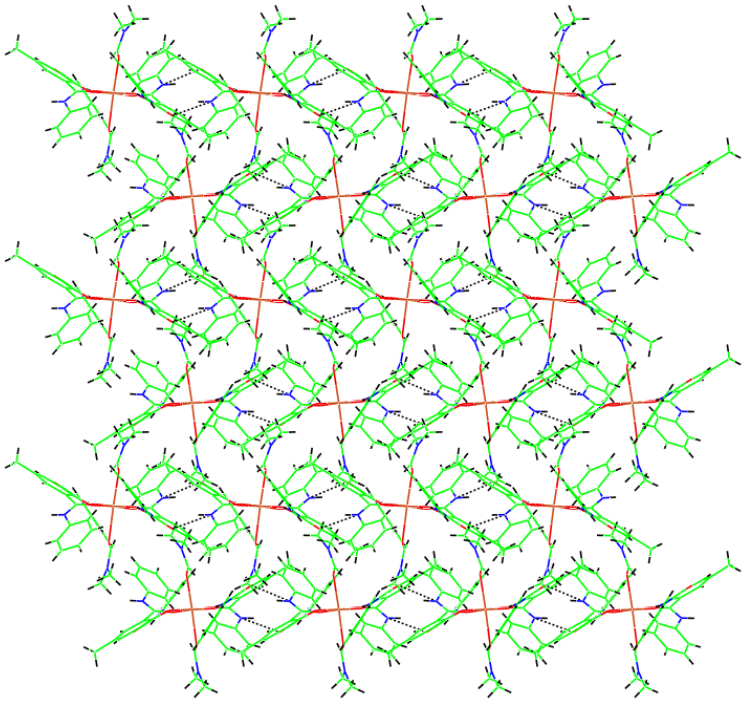


Fig. S5 A wireframe projection of the two dimensional sheet structure of $[CuL_2(dmf)_2]$ (**1**).

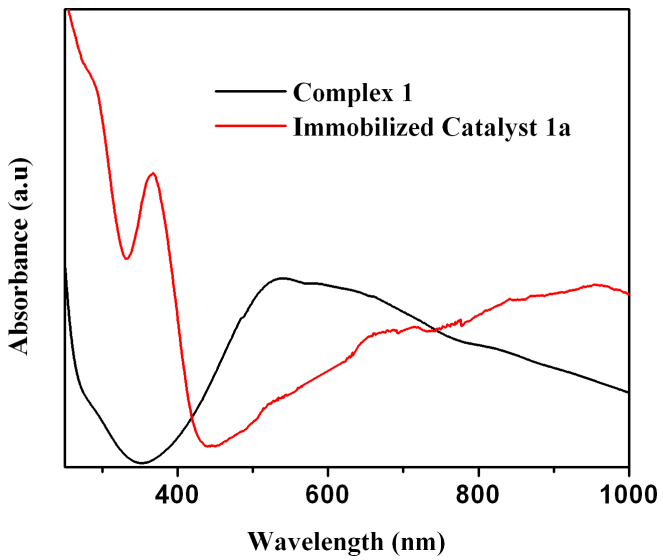


Fig. S6 UV-Vis-NIR spectrum of complex **1** and immobilized catalyst **1a** in solid state.

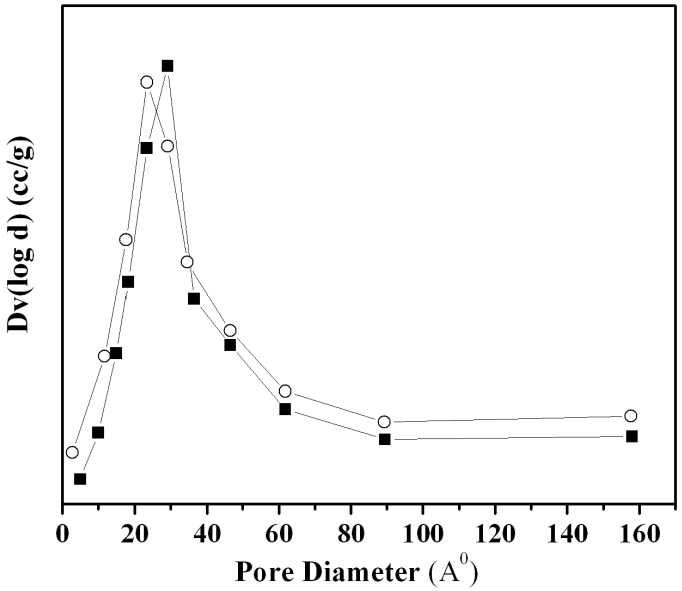


Fig. S7 Pore size distributions of mesoporous silica (■) and immobilized catalyst **1a** (○)**.**

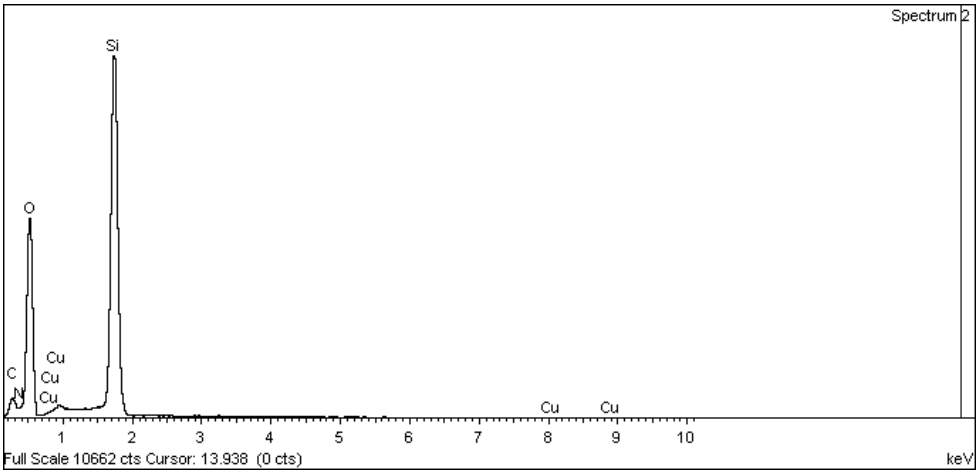
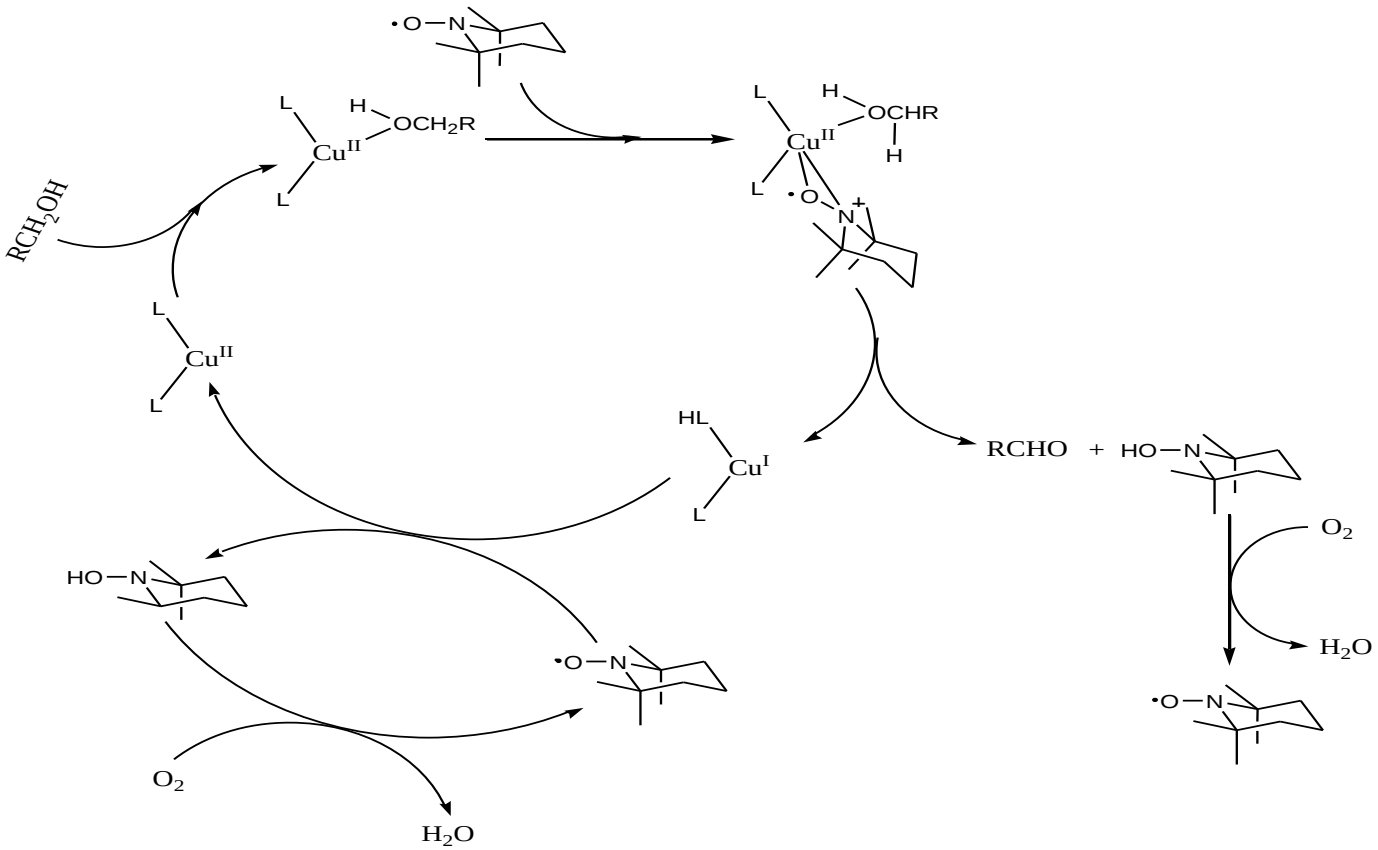


Fig. S8 EDS pattern of the catalyst **1a**.



Scheme S2 Proposed mechanism for catalytic aerobic oxidation of alcohols by immobilized catalyst 1a