Supplementary Information †

Structure, magnetism and catecholase activity of the first dicopper(II) complex having a single μ-alkoxo bridge

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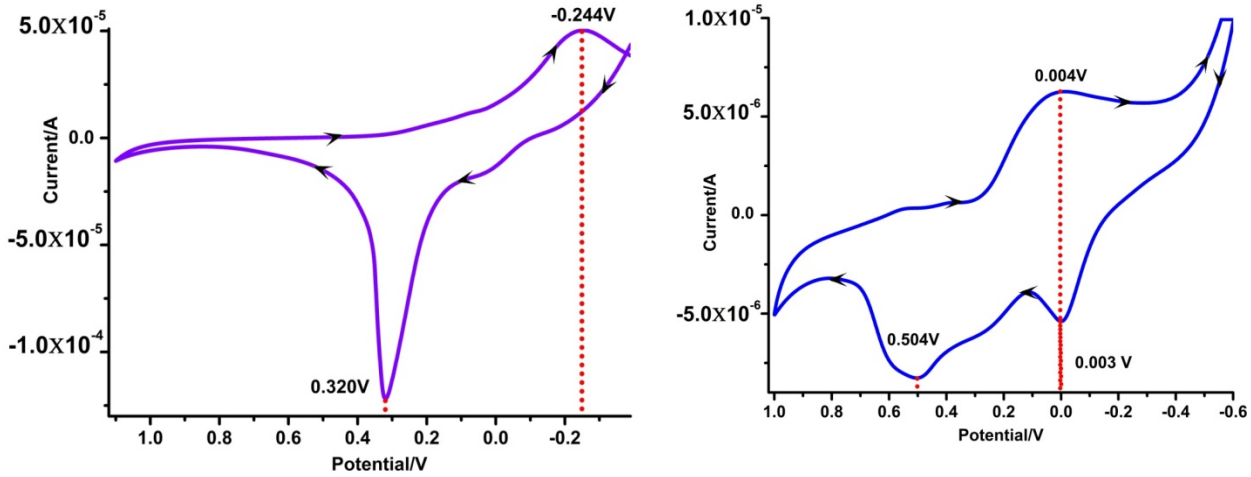
Table S1. Dependence of initial rates on the concentration of 3.5-DTBC, [conc. of Cu(II) complexes is $1x10^{-4}$ mol dm^{-3}].

[3,5-DTBC] (mol dm^{-3})	V (mol dm^{-3} s^{-1}) complex **1**	V (mol dm^{-3} s^{-1}) complex **2**
1E-3	7E-5	2.6049E-4
2E-3		3.564E-4
3E-3	1.34E-4	4.2946E-4
5E-3	1.68E-4	4.73E-4
7E-3	1.8949E-4	4.82E-4
1E-2	1.954E-4	5.013E-4

Table S2. Crystal data and structure refinement for **1** and **2**

	1	**2**
empirical formula	$C_{14}H_{17}CuN_2O_4 \cdot ClO_4$	$C_{35}H_{41}Cl_2Cu_3N_5O_{18}$
formula weight	440.29	1081.25
crystal system	Orthorhombic	Monoclinic
space group	*Fdd*2	$P2_1$
T (K)	100(2)	100(2)
a (Å)	27.107 (2)	11.1962(5)
b (Å)	42.977 (2)	15.1146(7)
c (Å)	11.7228 (8)	11.9446(5)
α (º)	90	90
β (º)	90	94.215(2)
γ (º)	90	90
Volume (Å^3)	13656.8 (16)	2015.87(15)
Z	32	2
μ. (mm^{-1})	1.48	1.787
reflections collected	41818	19831
independent reflections	6835 [R_{int} = 0.05]	19831 [R_{int} = 0.09]
data/restraints/parameters	41818/ 9 / 539	19831/ 1497 / 578
final R index [$I > 2\sigma(I)$]	R_1 = 0.0337, wR_2 = 0.0635	R_1 = 0.0525, wR_2 = 0.1168
final R index [*all data*]	R_1 = 0.0418, wR_2 = 0.0665	R_1 = 0.0698, wR_2 = 0.1314



Complex **1** Complex **2**

Fig. S1 Cyclic voltammogram of complexes **1** and **2** in MeOH using 0.1 M TBAP as supporting electrolyte and platinum working electrode (scan rate 100 mVs^{-1}).

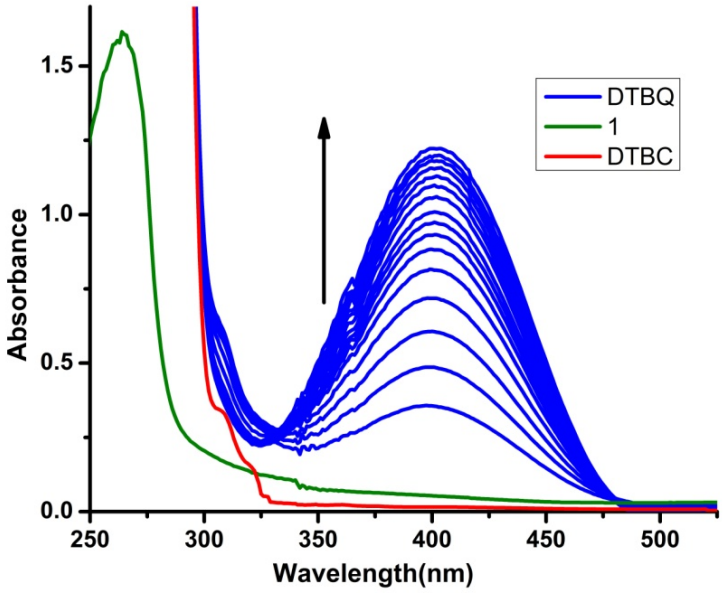


Fig. S2 Increase in the quinone band at 400 nm after addition of 100 fold 3,5-DTBC (1×10^{-2} M) to the methanol solution of complex **2** (1×10^{-4} M). The spectra are recorded at an interval of 5 min.

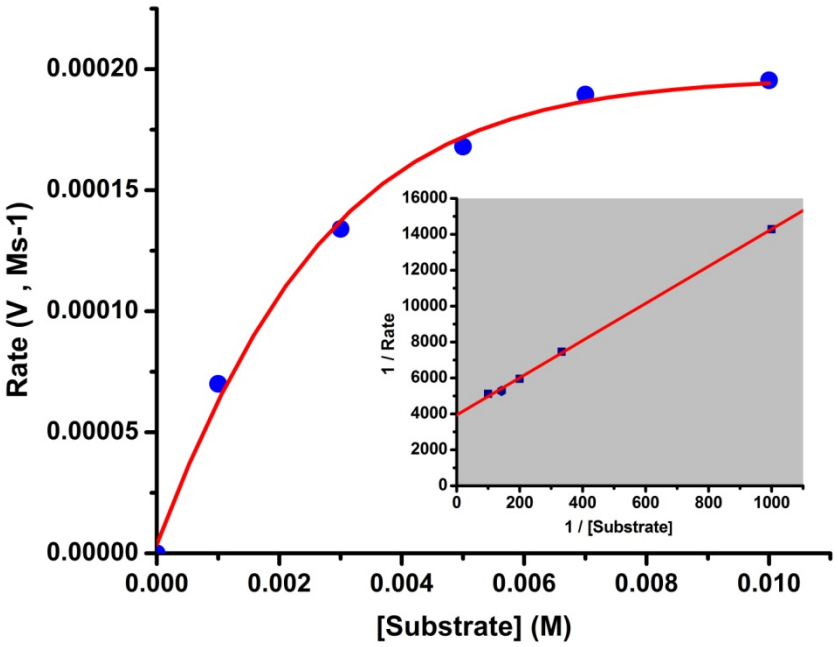


Fig. S3 Plot of rate *vs.* substrate concentration for complex **1**. Inset shows Lineweaver–Burk plot.

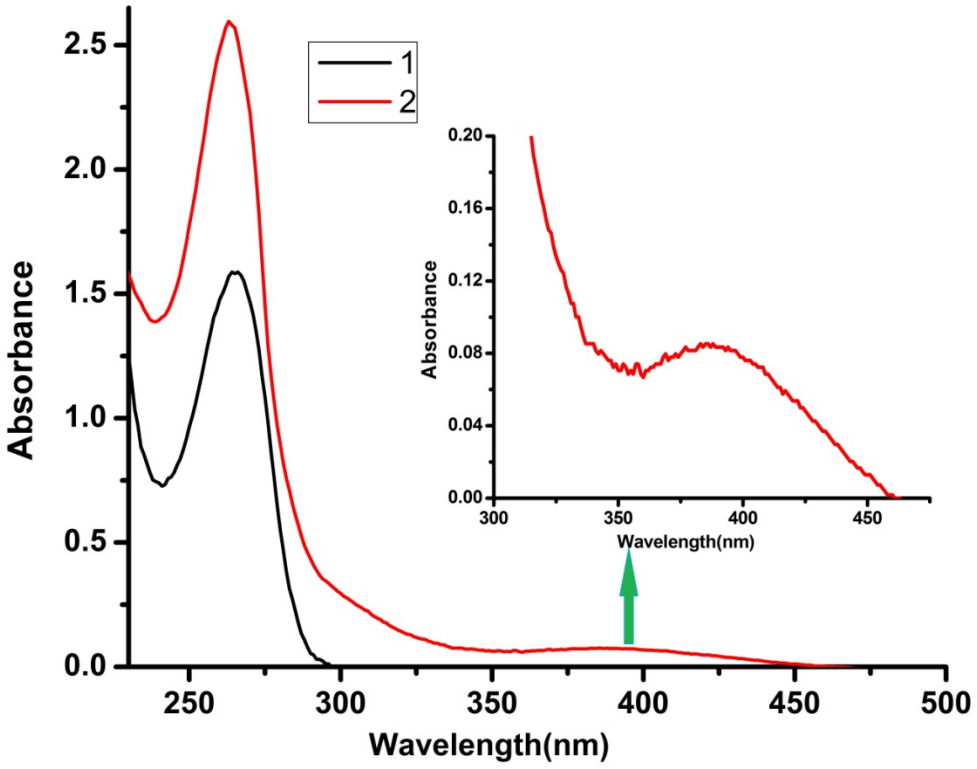


Fig. S4 UV-Vis spectra of complex **1** and **2** in MeOH ([**1**] = 1 x 10^{-4} M)

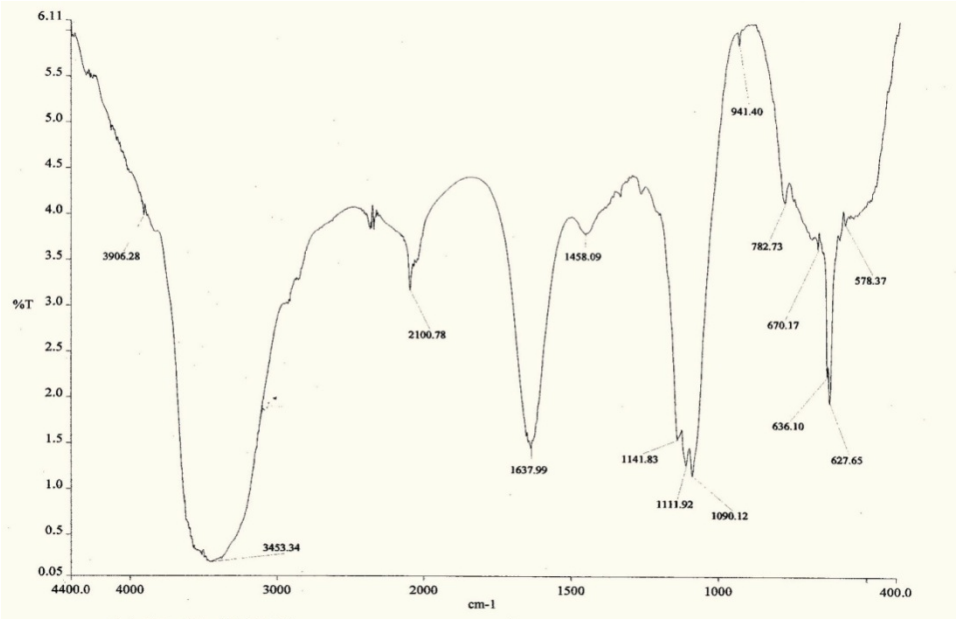


Fig. S5 FTIR spectrum of **1**

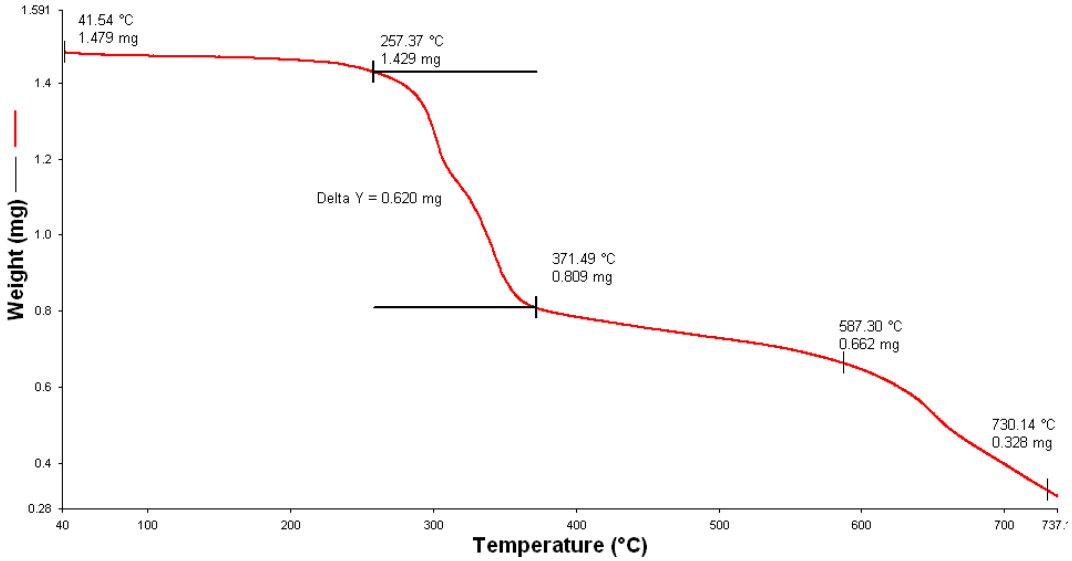


Fig. S6 Thermogram of **1**

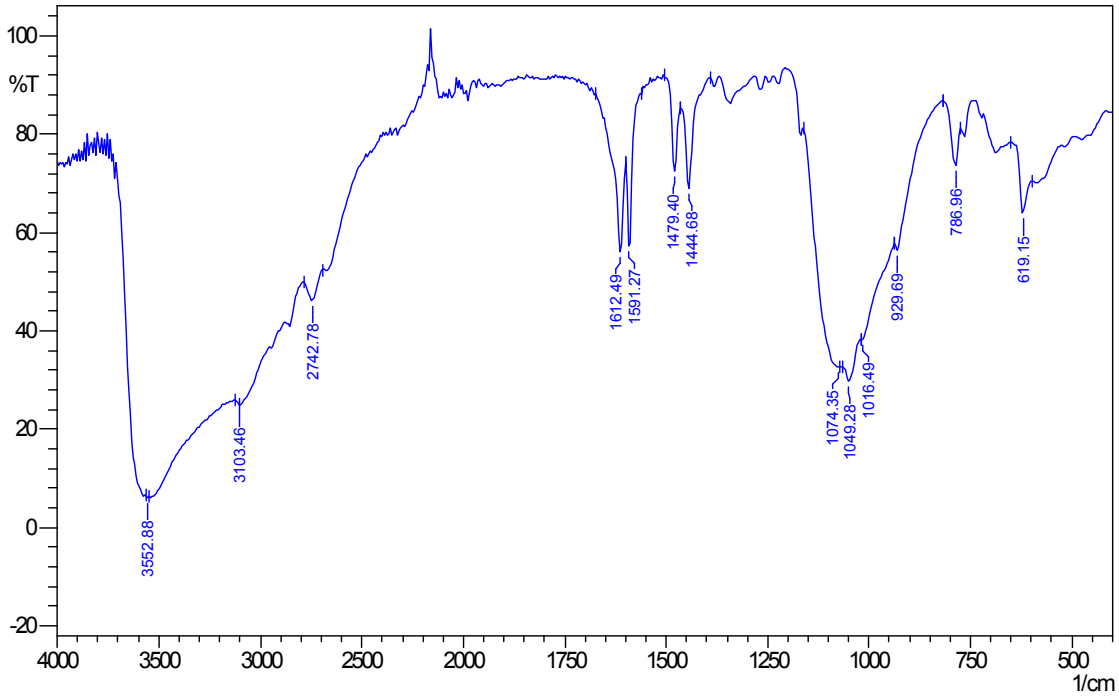


Fig. S7 FTIR spectrum of **2**

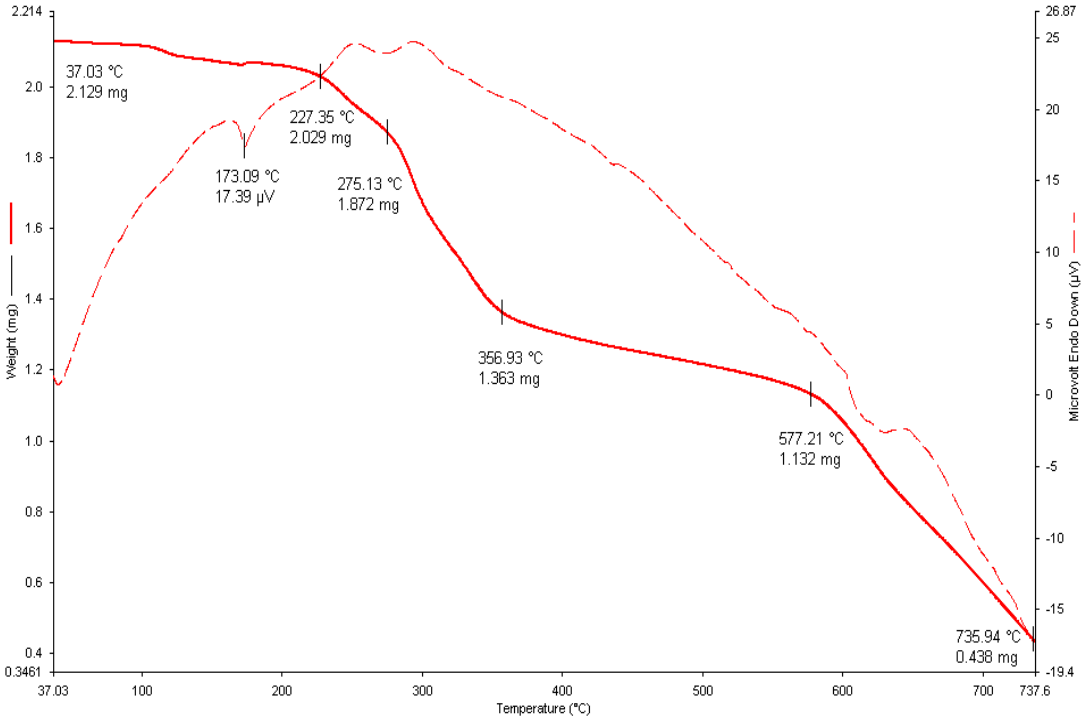


Figure S8 Thermogram of **2**