Electronic Supplementary Information

A mononuclear cobalt(III) complex and its catecholase activity

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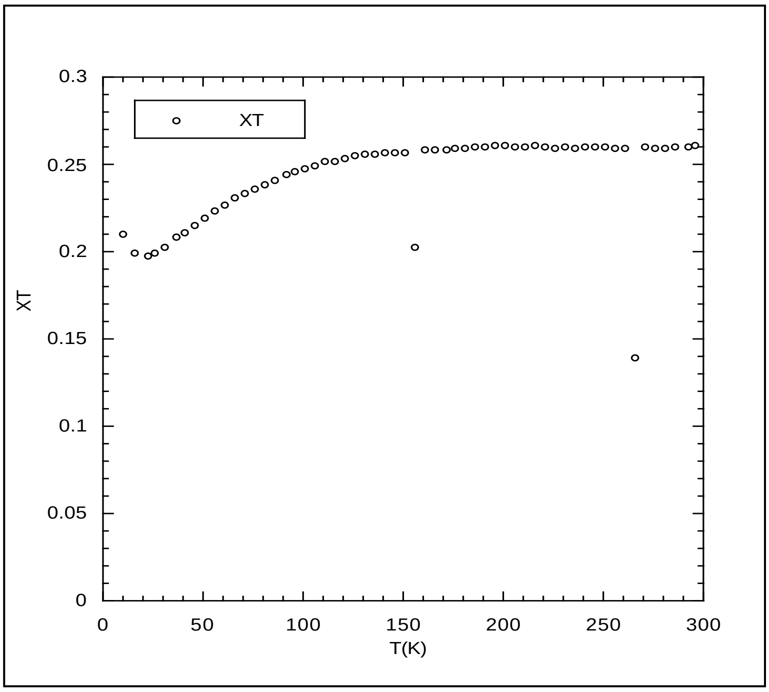


Fig. S1 χT vs. T plot of complex **1** showing diamagnetic behaviour.

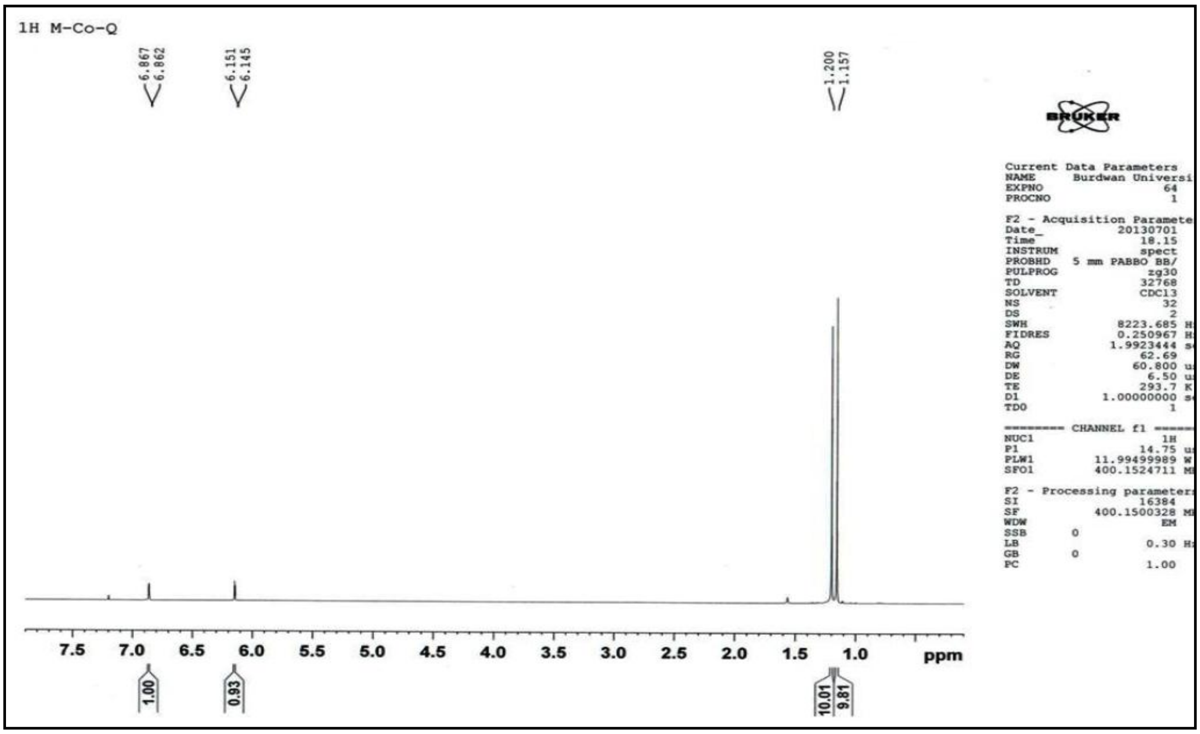


Fig. S2 ^{1}H NMR spectrum of 3,5-DTBQ in $CDCl_3$.

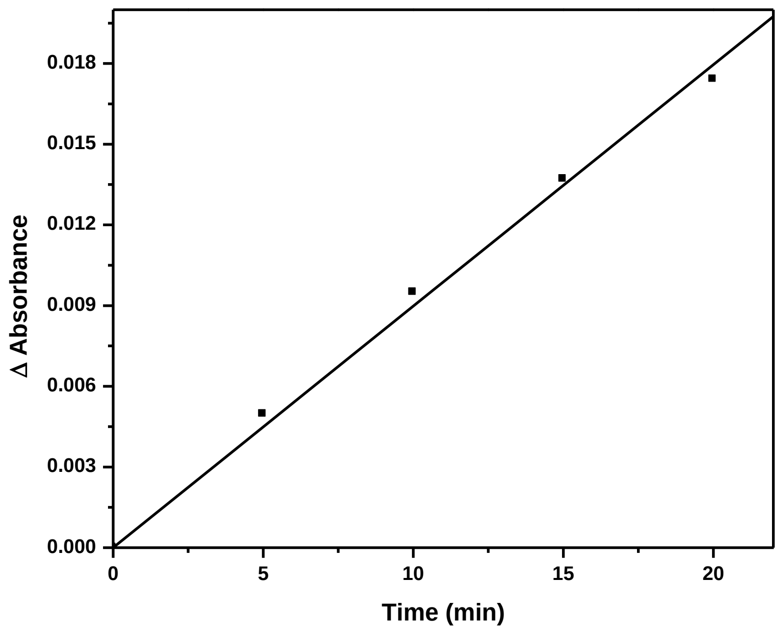


Fig. S3 A plot of the difference in absorbance (ΔA) vs time to evaluate the initial rate of the catalysis by **1** in MeOH.

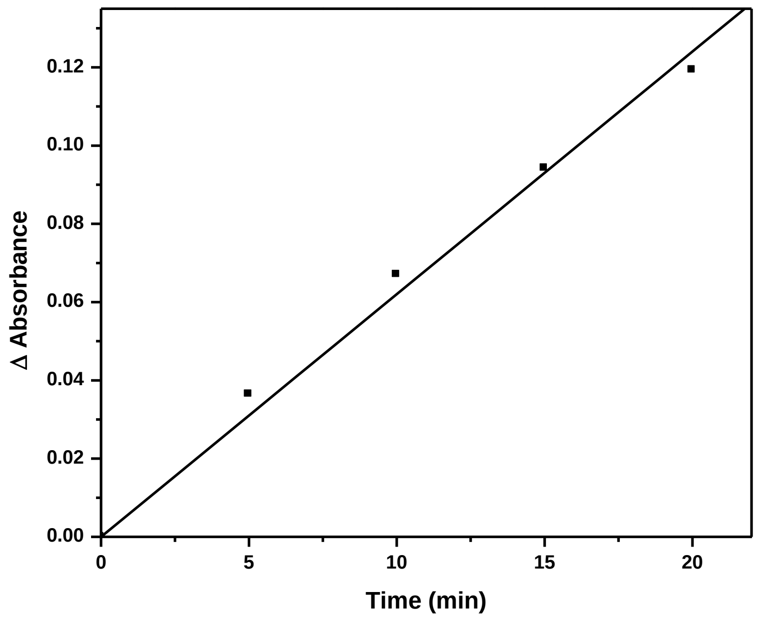


Fig. S4 A plot of the difference in absorbance (ΔA) vs time to evaluate the initial rate of the catalysis by **1** in MeCN.

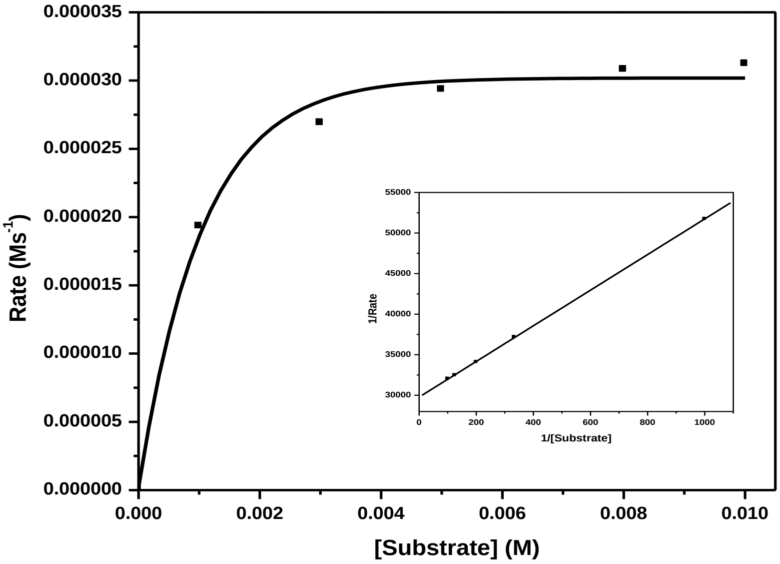


Fig. S5 Plot of rate vs. [substrate] in presence of **1** in MeOH; inset: Lineweaver-Burk plot**.**

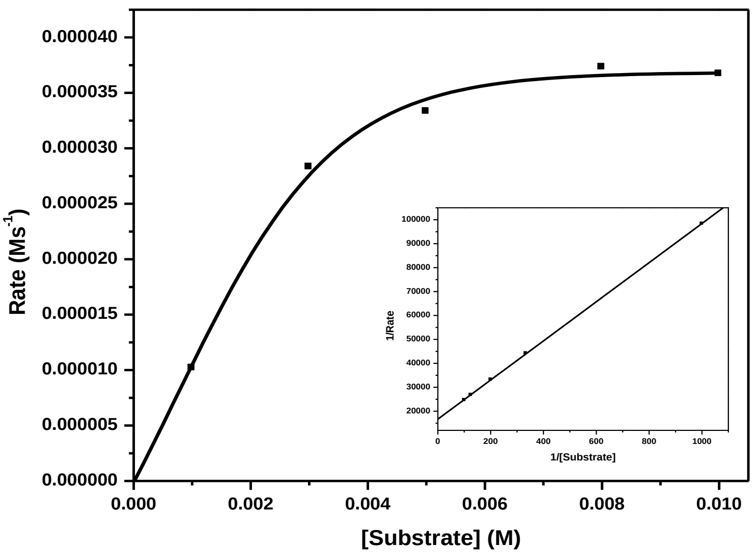


Fig. S6 Plot of rate vs. [substrate] in presence of **1** in MeCN; inset: Lineweaver-Burk plot.

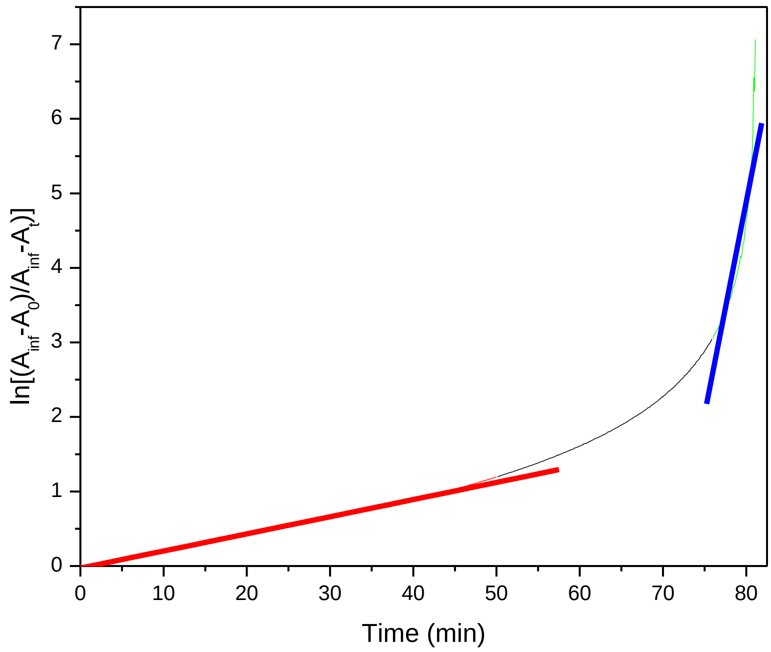


Fig. S7 Rate plot showing two-step mechanistic pathway of the catalytic process.

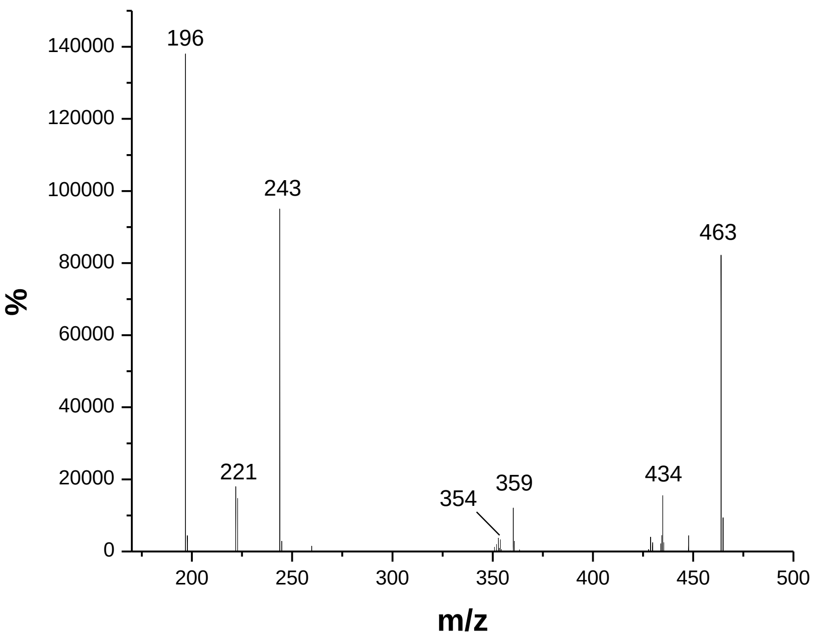
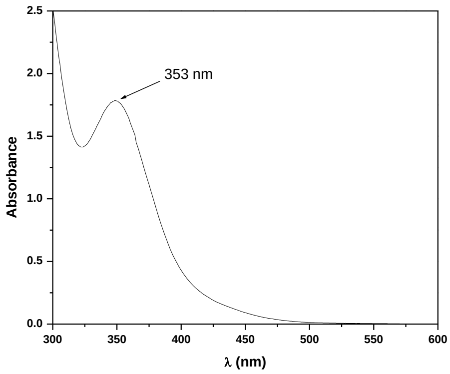


Fig. S8 ESI-MS spectrum of a 1:100 mixture of **1** and 3,5-DTBC in MeOH.

S1. Spectrophotometric detection of H_2O_2 in the oxidation reaction[19]

Reaction mixtures were prepared as in the kinetic experiments. After 1 h of reaction an equal volume of water was added and the quinone formed was extracted three times with dichloromethane. The aqueous layer was acidified with H_2SO_4 to pH =2 to stop further oxidation, and 1 mL of a 10% solution of KI and three drops of 3% solution of ammonium molybdate were added. In the presence of hydrogen peroxide occurs the reaction $H_2O_2 + 2I^- + 2H^+ \rightarrow 2H_2O + I_2$, and with an excess of iodide ions, the triiodide ion is formed according to the reaction $I_2(aq) + I^- \rightleftharpoons I^{3-}$. The formation of I^{3-} was monitored spectrophotometrically due to the development of the characteristic I^{3-} band (λ = 353 nm, ε = 26000 M^{-1} cm^{-1}).



S2. Spectrophotometric determination of concentration of O_2

Spectrophotometrically we have determined the absorbance of I^{3-} to be 1.797. Therefore, its concentration is 6.9115×10^{-5} (M). From the above equations, discussed in **S1**,

1 equivalent I^{3-} = 1 equivalent I_2

380.7 I^{3-} is equivalent to 253.8 I_2

Therefore, 6.9115×10^{-5} (M) I^{3-} is equivalent to 4.60766×10^{-5} (M) I_2

1 equivalent I_2 = 1 equivalent H_2O_2

253.8 I_2 is equivalent to 34.02 H_2O_2

Therefore, 4.60766×10^{-5} (M) I_2 is equivalent to 6.1762×10^{-6} (M) H_2O_2

1 equivalent H_2O_2 = 1 equivalent O_2

34.02 H_2O_2 is equivalent to 32.0 O_2

Therefore, 6.1762×10^{-6} (M) H_2O_2 is equivalent to 5.8095×10^{-6} (M) O_2