Electronic Supplementary Material (ESI) for Dalton Transactions.


# Electronic Supporting Information

For the manuscript entitled

**Copper based coordination polymers based on metalloligands: Utilization as the heterogeneous oxidation catalysts**

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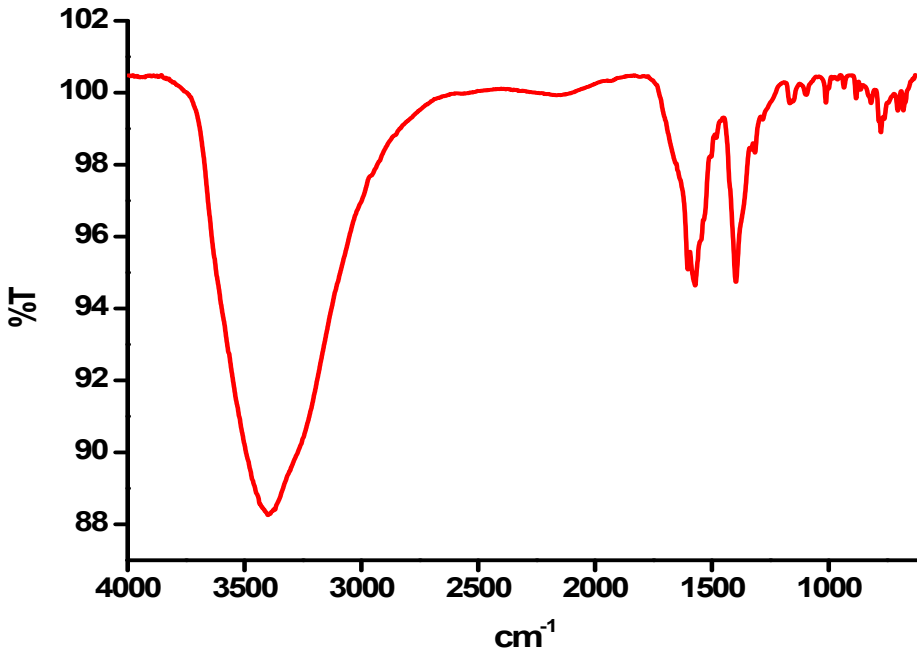


Figure S1. FTIR spectrum of **1-Cu**.

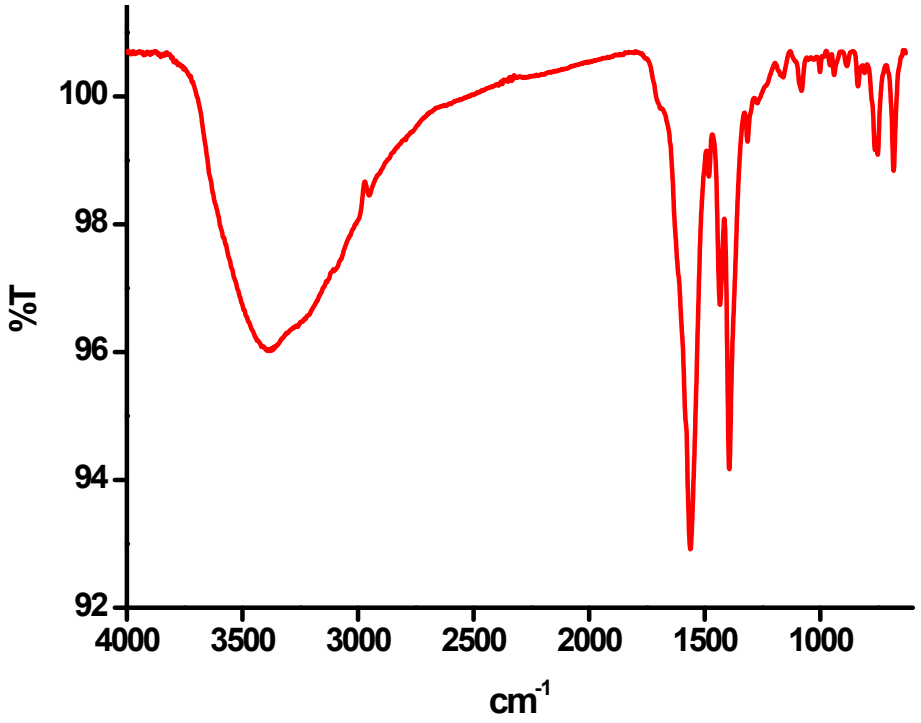


Figure S2. FTIR spectrum of **2-Cu**.

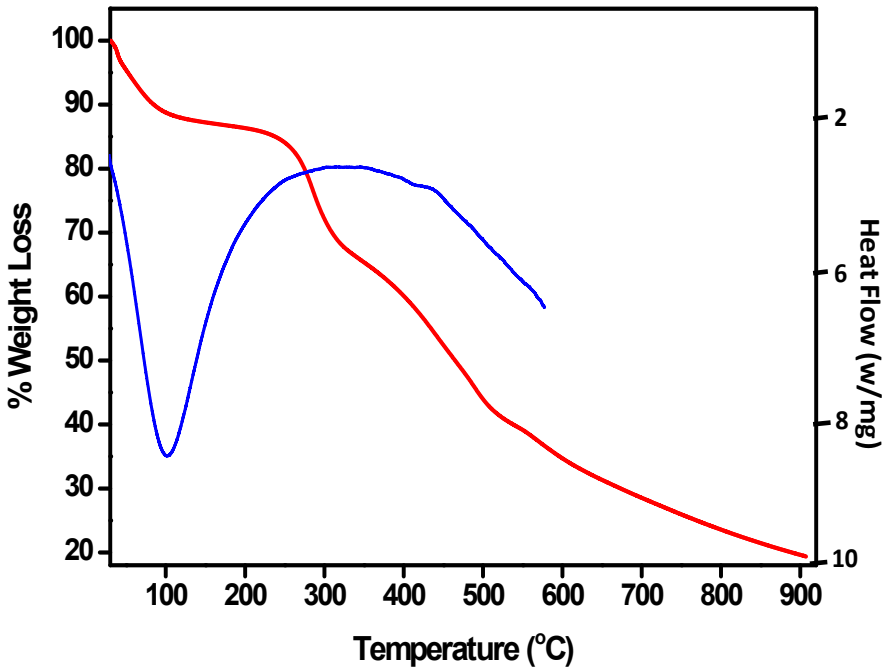


Figure S3. Thermal Gravimetric Analysis (TGA, red trace) and Differential Scanning Calorimetric (DSC, blue trace) plots for **1-Cu**.

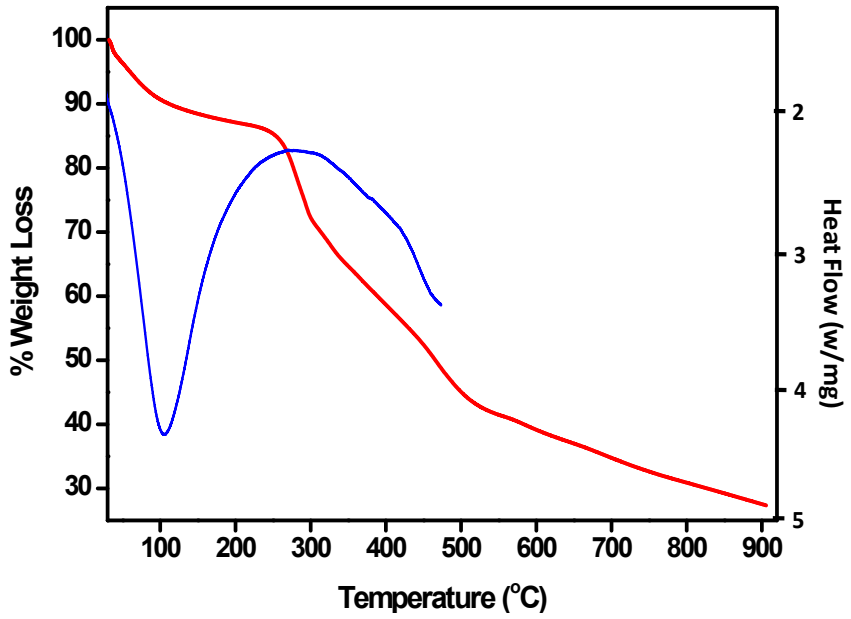


Figure S4. Thermal Gravimetric Analysis (TGA, red trace) and Differential Scanning Calorimetric (DSC, blue trace) plots for **2-Cu**.

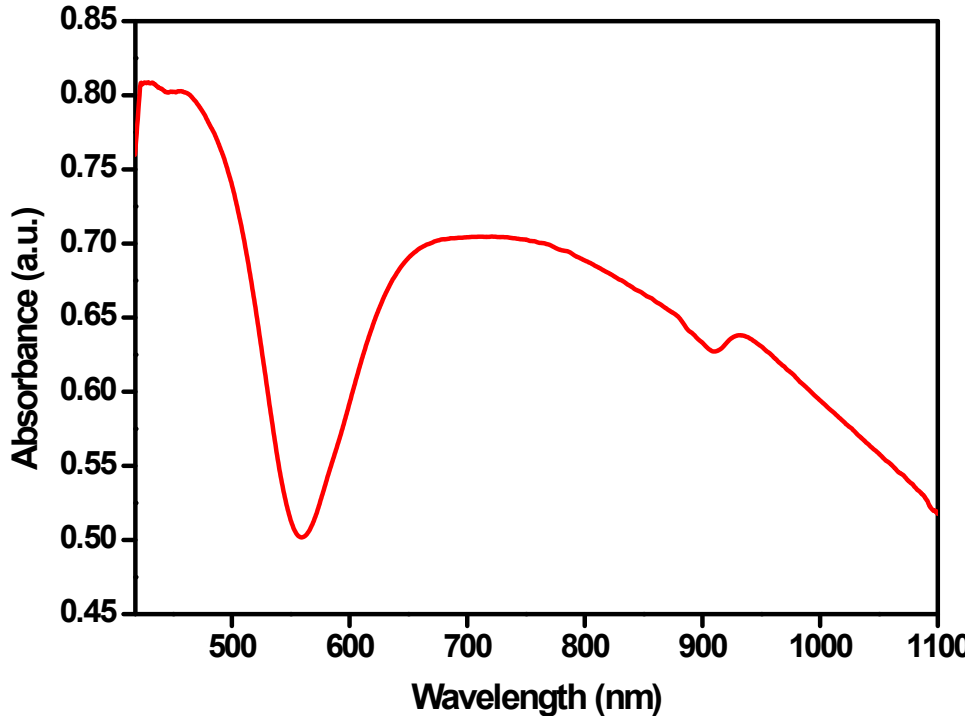


Figure S5. Diffuse reflectance UV-Vis spectrum of **1-Cu**.

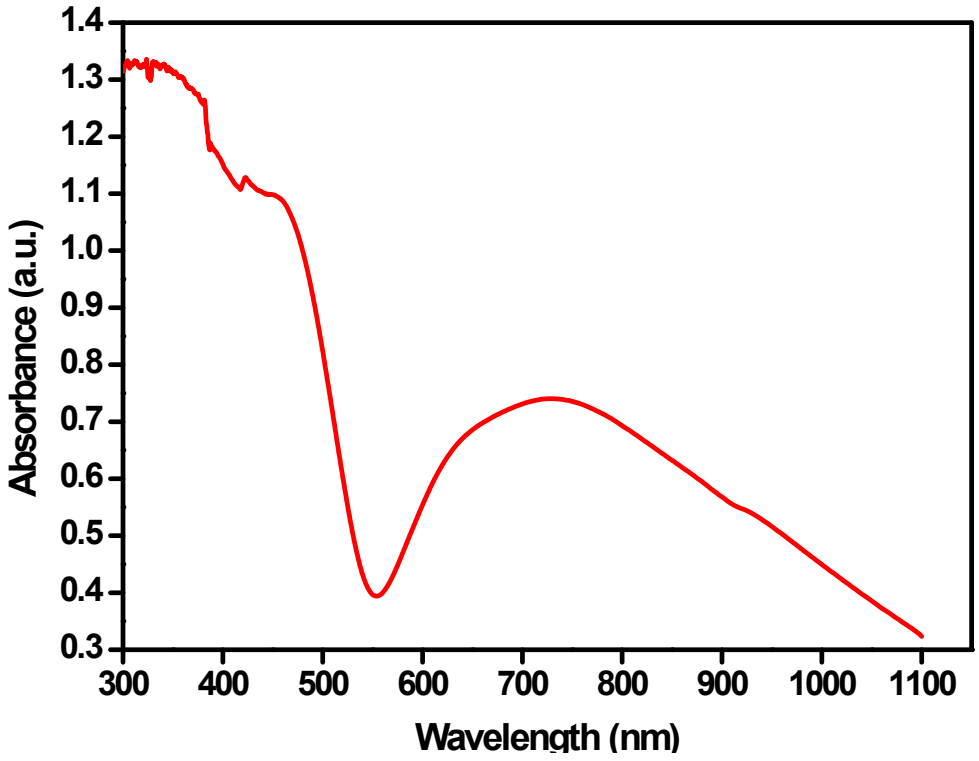


Figure S6. Diffuse reflectance UV-Vis spectrum of **2-Cu**.

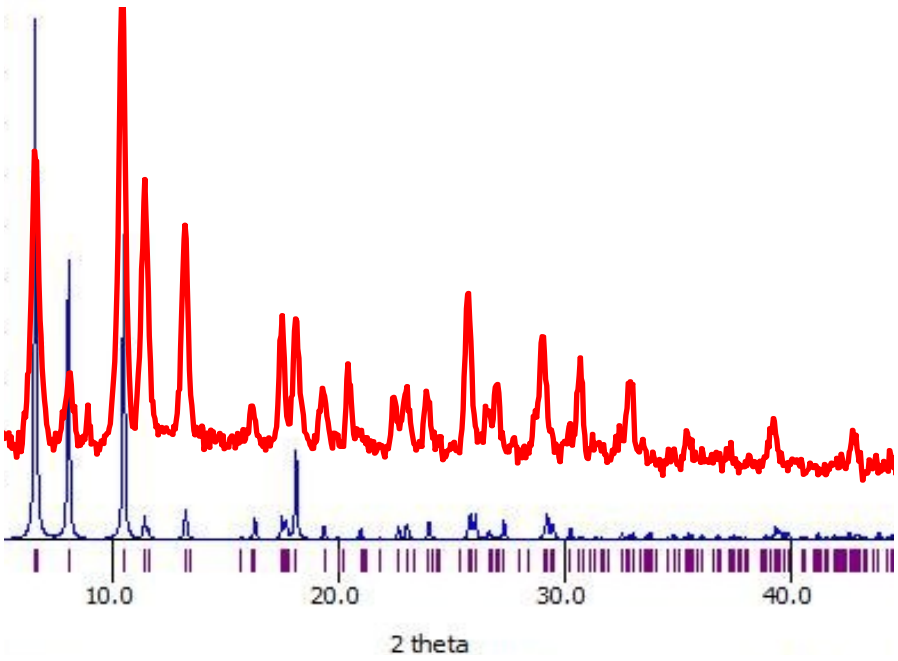


Figure S7A. X-ray Powder Diffraction (XRPD) patterns for as-synthesized **1-Cu** (red trace) and the one simulated from mercury 3.8 using single crystal diffraction data.

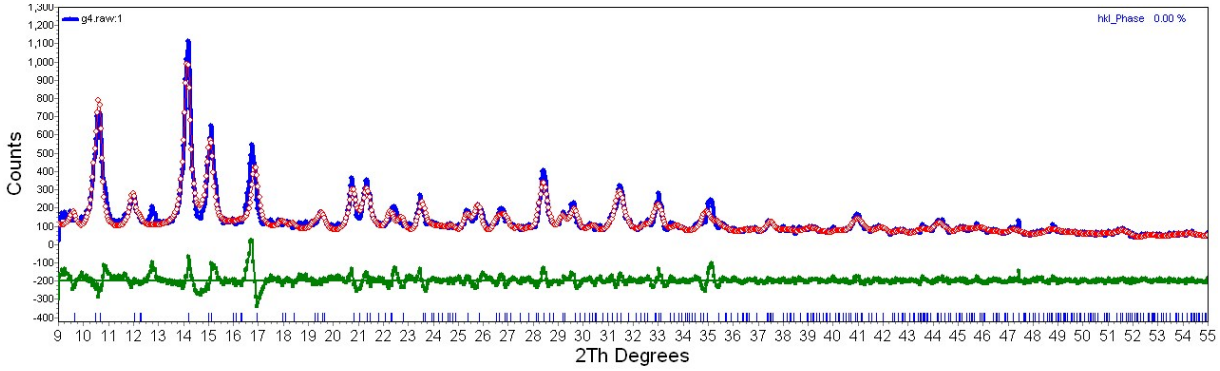


Figure S7B. Le Bail refinement of X-ray powder diffraction (XRPD) pattern of **1-Cu**. The observed, calculated (profile matching) and difference profiles are given in blue, red, and olive lines, respectively. Generated Bragg positions are provided as blue vertical lines.

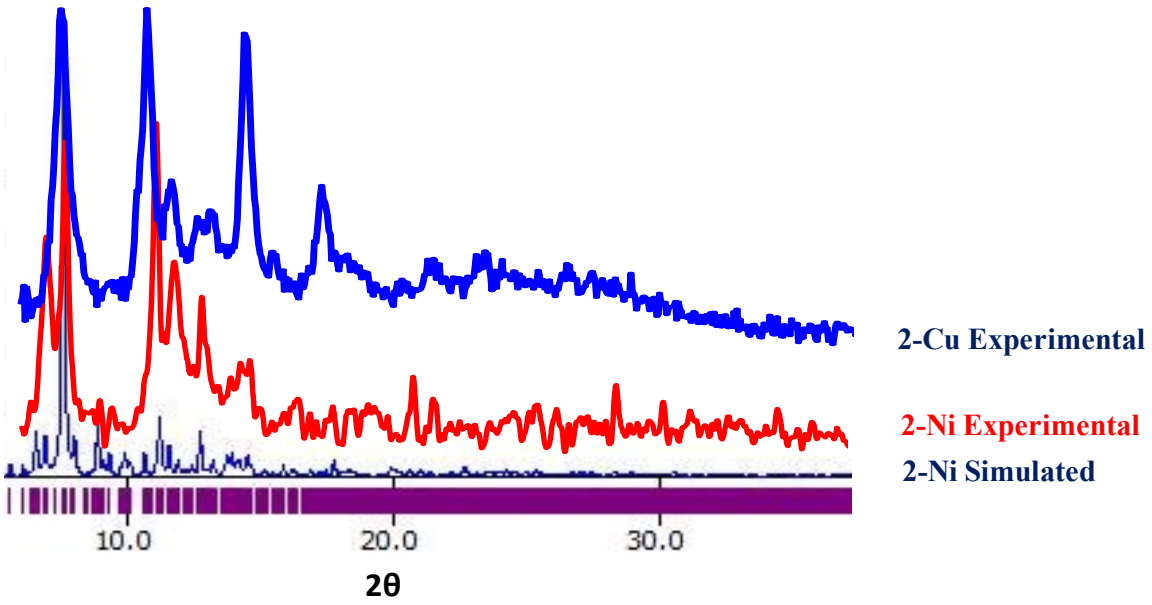


Figure S8A. X-ray Powder Diffraction (XRPD) patterns for as-synthesized **2-Cu** (blue trace) and its comparison with our earlier reported coordination polymer, **2-Ni** (red trace).

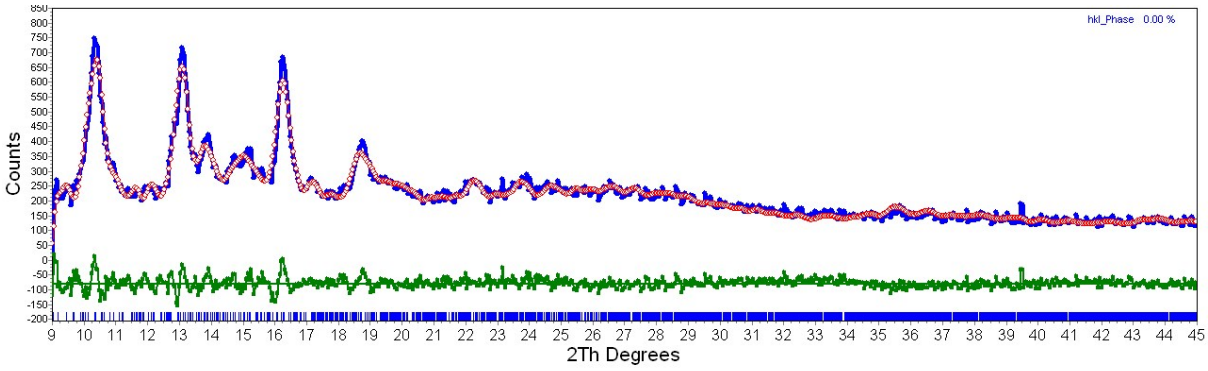


Figure S8B. Le Bail refinement of X-ray powder diffraction (XRPD) pattern of **2-Cu** using single crystal diffraction data for our earlier reported coordination polymer, **2-Ni**. The observed, calculated (profile matching) and difference profiles are given in blue, red, and olive lines, respectively. Generated Bragg positions are provided as blue vertical lines.

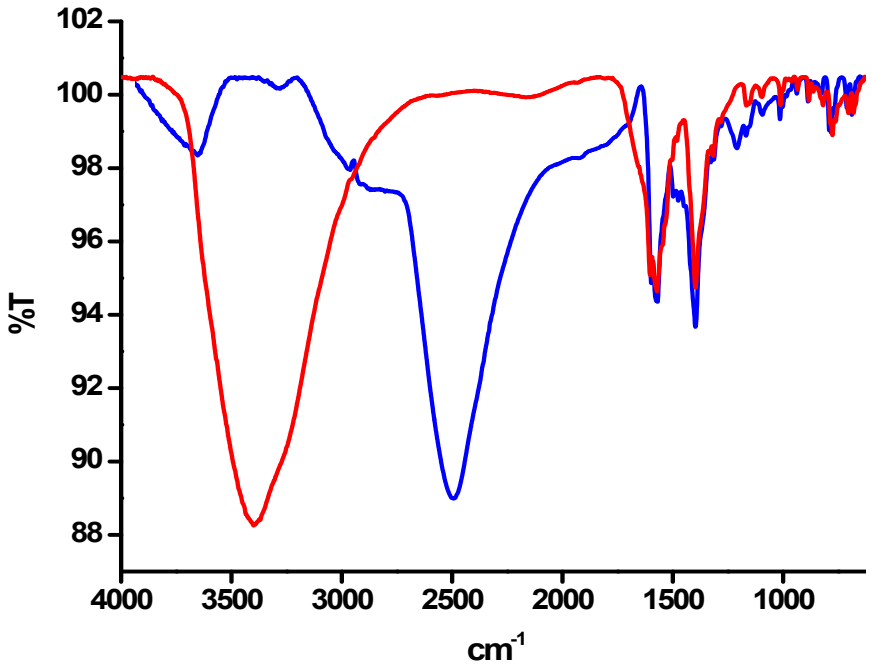


Figure S9. FTIR spectra of as synthesized **1-Cu** (red trace) and after $D_2O$ exchange experiment (blue trace).

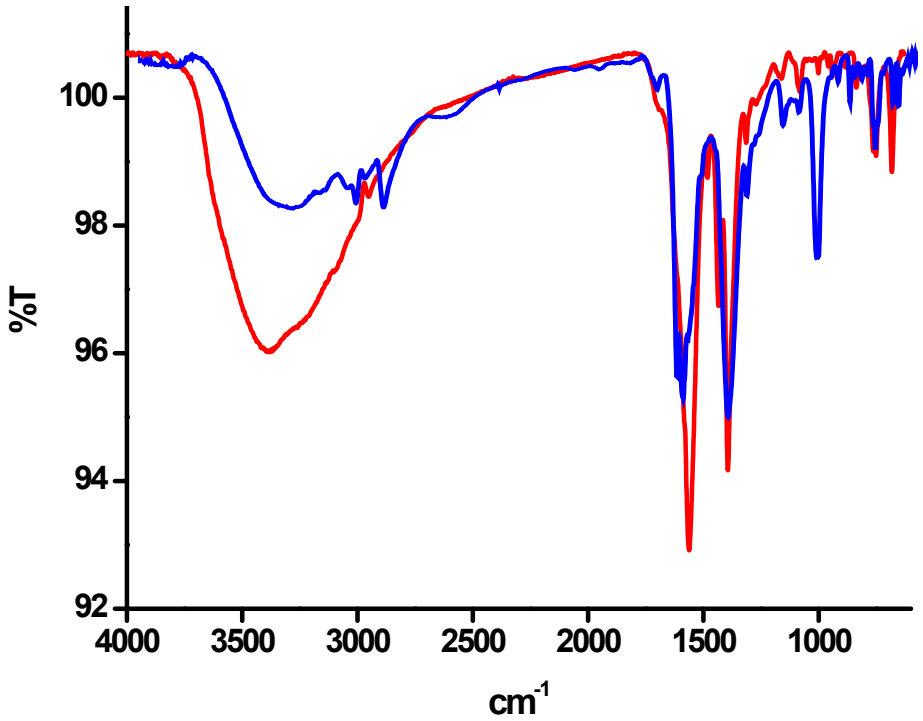


Figure S10. FTIR spectra of as synthesized **1-Cu** (red trace) and after methanol exchange experiment (blue trace).

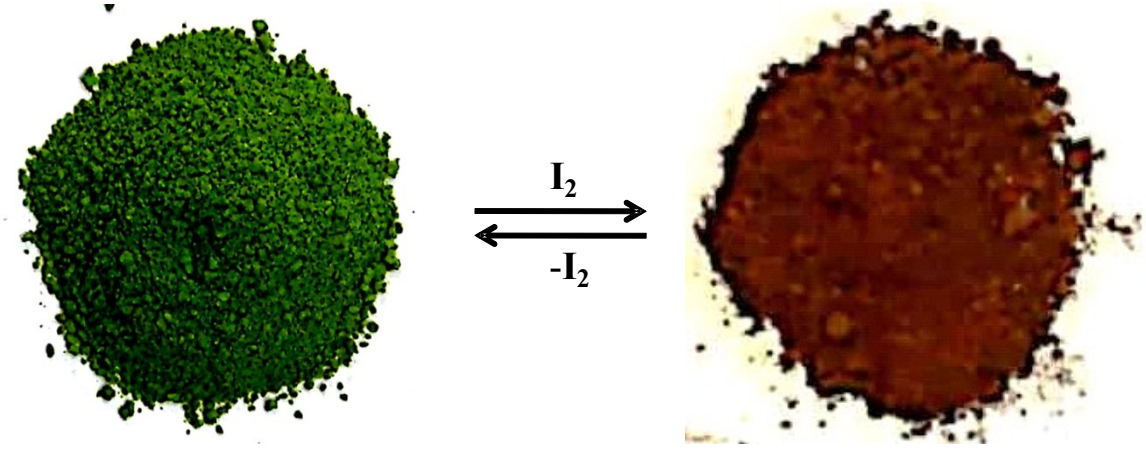


Figure S11. Optical images of a solid sample of (a) as synthesized **1-Cu** and (b) after molecular iodine adsorption experiment.

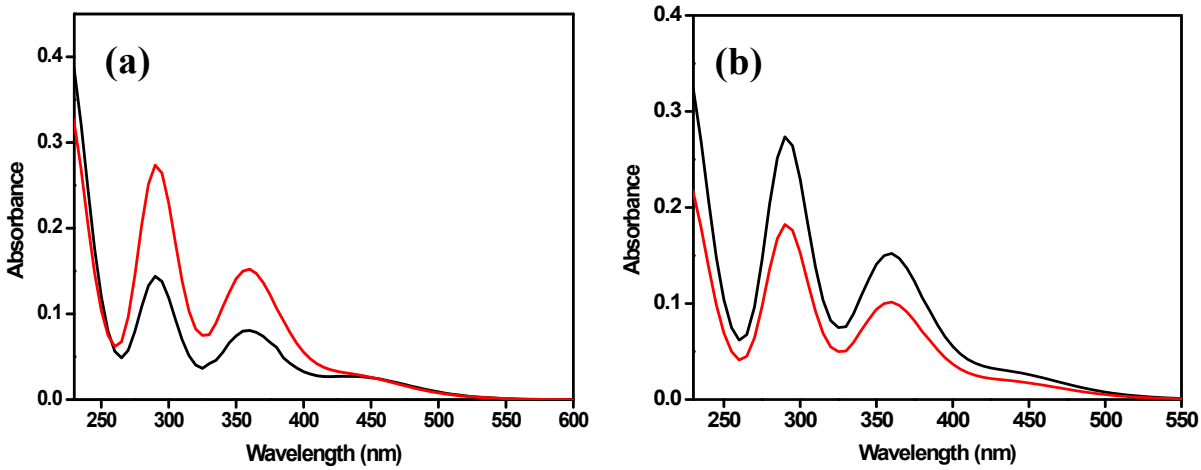


Figure S12. (a) UV-Vis spectrum of standard triiodide ion (red trace) and triiodide ion generated by **1-Cu** in MeOH solution of KI (black trace). (b) UV-Vis spectrum of standard triiodide ion (black trace) and triiodide ion generated by **2-Cu** in MeOH solution of KI (red trace).

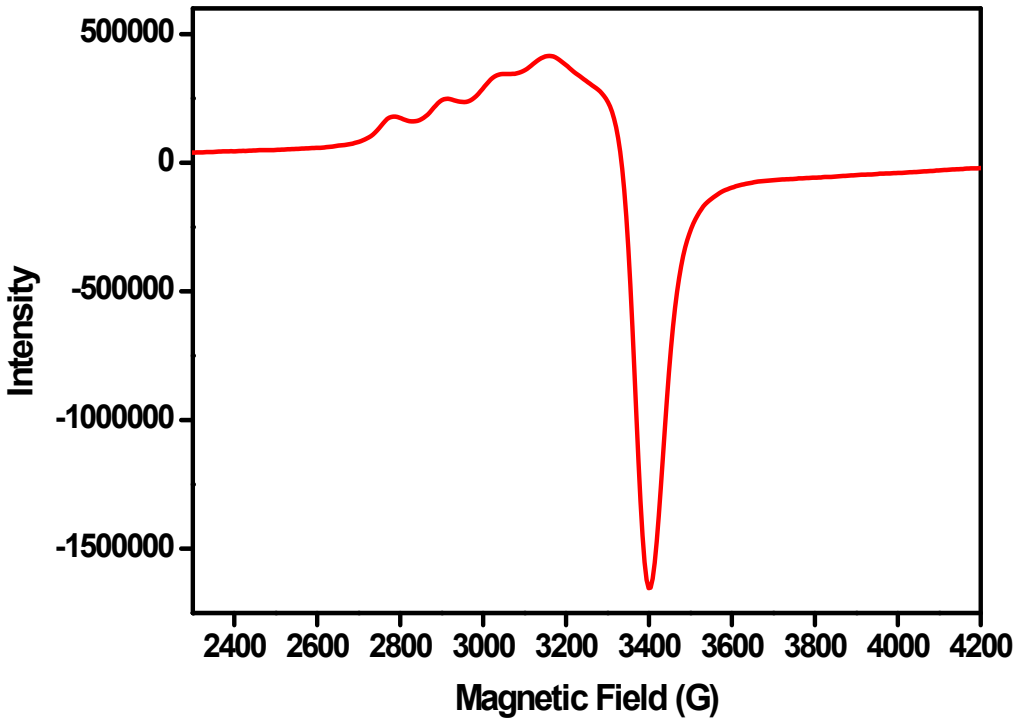


Figure S13. Solid-state EPR spectrum of powdered **1-Cu**.

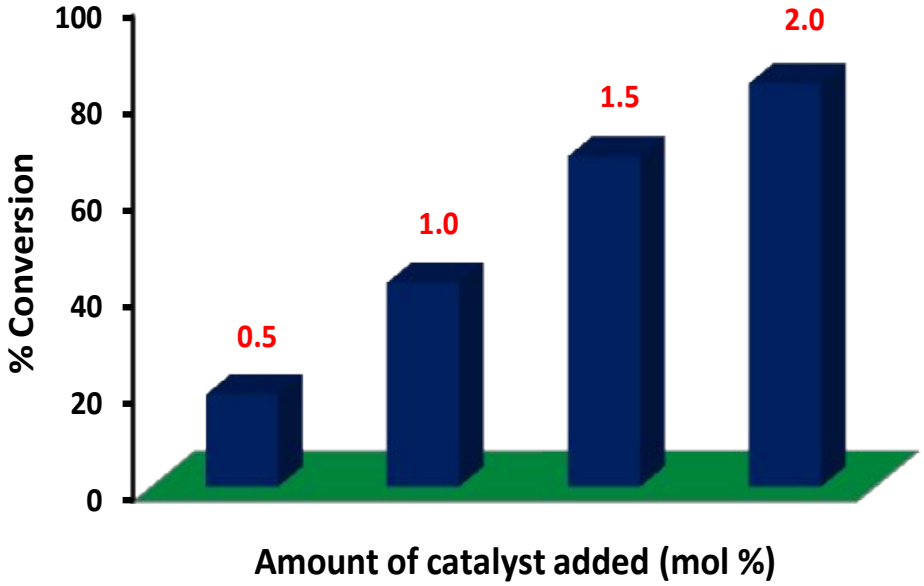


Figure S14. Effect of catalyst loading (**1-Cu**) on the epoxidation of styrene using molecular oxygen and isobutyraldehyde.

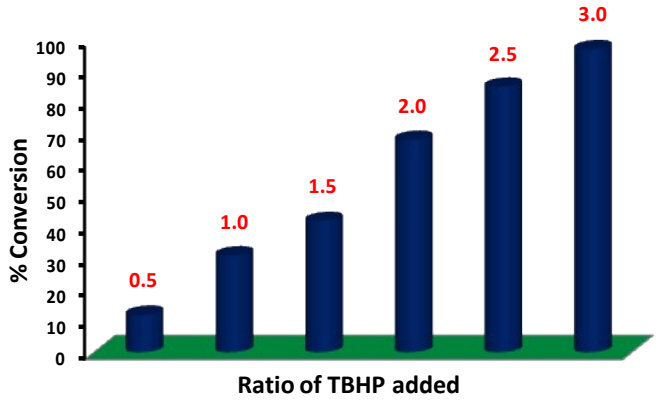


Figure S15. Effect of ratio of TBHP on the oxidation of benzyl alcohol using **1-Cu** as a catalyst.

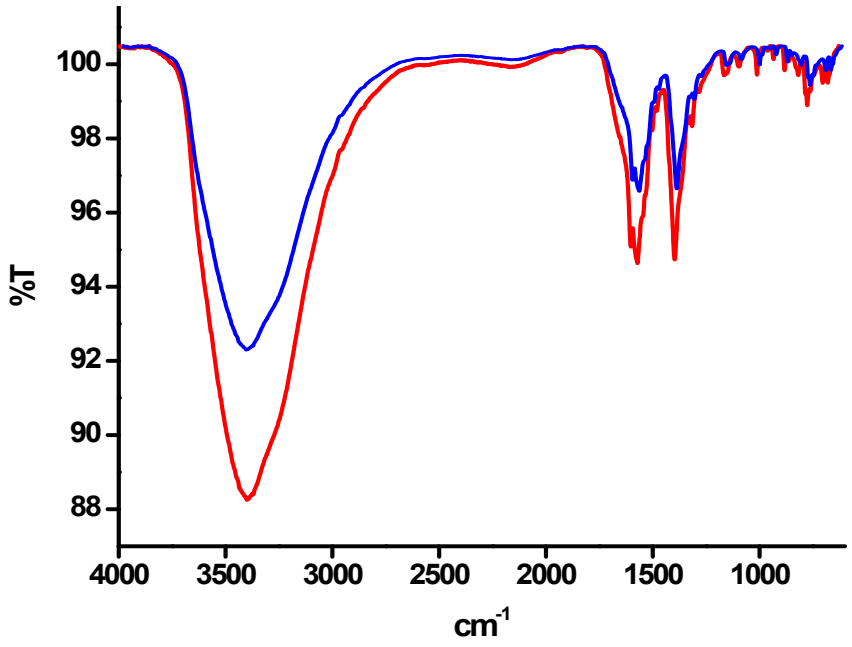


Figure S16. FTIR spectra of as-synthesized **1-Cu** (red trace) and the one recovered after oxidation of benzyl alcohol using TBHP (blue trace).

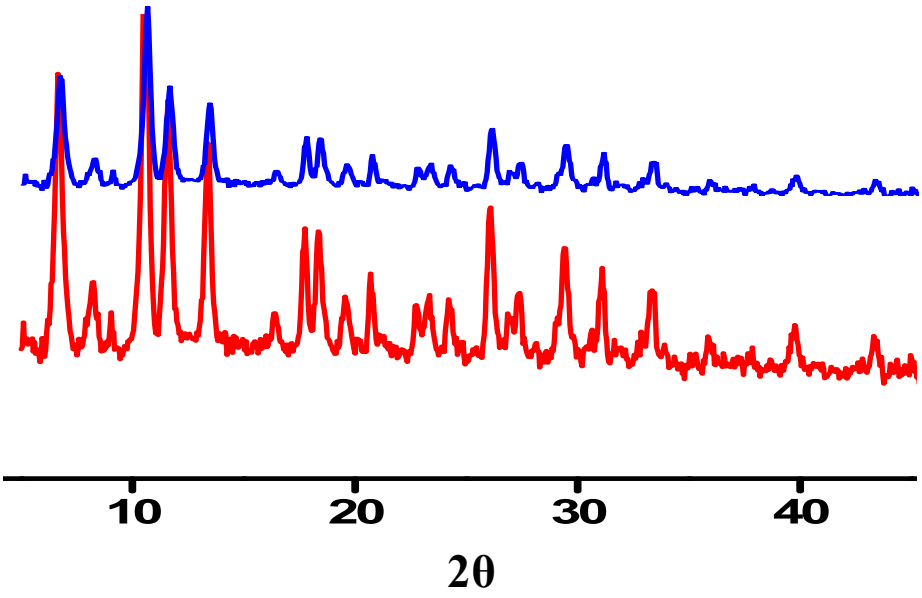


Figure S17. X-ray Powder Diffraction (XRPD) patterns for as-synthesized **1-Cu** (red trace) and the one recovered after oxidation of benzyl alcohol using TBHP (blue trace).

**Table S1.**Crystallographic data collection and structure refinement parameters for **1-Cu**.

| | **1-Cu** |
|---|---|
| Empirical formula | $C_{21}H_{11}Co_{0.50}Cu_{0.58}N_3O_{10.25}$ |
| Formula weight | 535.41 |
| T (K) | 293(2) K |
| Crystal system | Tetragonal |
| Space group | *I* 4/m |
| *a* (Å) | 15.440(5) |
| *b* (Å) | 15.440(5) |
| *c* (Å) | 26.265(5) |
| $\alpha = \beta = \gamma$ (˚) | 90 |
| *V* (Å)$^3$ | 6261(4) |
| *Z* | 8 |
| *d* (g cm$^{-3}$) | 1.136 Mg/m3 |
| $\mu$ (mm$^{-1}$) | 0.719 |
| *F* (000) | 2162 |
| *R* (int.) | 0.0603 |
| Final *R* indices[a] | $R_1 = 0.0691$ |
| [$I>2\sigma(I)$] | $wR_2 = 0.2038$ |
| *R* indices | $R_1 = 0.0759$ |
| All data | $wR_2 = 0.2080$ |
| GOF on $F^2$ | 1.128 |
| CCDC No. | 1869008 |

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b]$wR_2 = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2]/\Sigma[wF_o^4]\}^{1/2}$.