Electronic Supplementary Information for

The impact of Copper source on the synthesis of meso-structured CuTUD-1: A promising catalyst for phenol hydroxylation

Muthusamy Poomalai Pachamuthu,[a] Vinju Vasudevan Srinivasan,[a] Rajamanickam Maheswari,[a, b] Kannan Shanthi[a]* and Anand Ramanathan[b]*

[a] *Department of Chemistry, Anna University, Chennai 600025, India, Tel.: +91-9840146642; E-Mail: kshanthiramesh@yahoo.com (K.S)*

[b]*Center for Environmentally Beneficial Catalysis (CEBC), The University of Kansas, Lawrence, KS 66047, USA, Tel.: +1-785-864-1631; Fax: +1-785-864-6051; E-mail: anand@ku.edu*

Estimation of phenol conversion and products selectivity over CuTUD-1 catalysed Phenol hydroxylation:

Since water is used as the solvent, finding a suitable internal standard was difficult and hence internal standards were used. However, the concentration of reactants and products were varied and an area calibration was carried out to arrive at exact conversion and selectivity of products.

- The concentration of phenol was determined using the equations given below.

  $X_{phenol}(\%)$ = (Initial Cp – Final Cp)/ Initial Cp X 100

  Cp is the molar concentration of phenol.

- The selectivity of products catechol (CC), hydroquinone (HQ) and benzoquinone (BQ) are calculated

  $S_{CC}(\%)$ = Initial C_{CC} / (Initial Cp – Final Cp) X 100

  $S_{HQ}(\%)$ = Initial C_{HQ} / (Initial Cp – Final Cp) X 100

  $S_{BQ}(\%)$ = Initial C_{BQ} / (Initial Cp – Final Cp) X 100

  Where C_{cc}, C_{HQ} and C_{BQ} are molar concentrations of catechol (CC), hydroquinone (HQ) and benzoquinone (BQ) respectively.

- The conversion of H_2O_2 is determined the equation

  $X_{H2O2}(\%)$: (Initial C_{H2O2} – Final C_{H2O2})/ Initial C_{H2O2} X 100

  C_{H2O2} is the molar concentration of H_2O_2

Iodometry titration method adopted to estimate the molar concentration of H_2O_2 present in the reaction mixture.

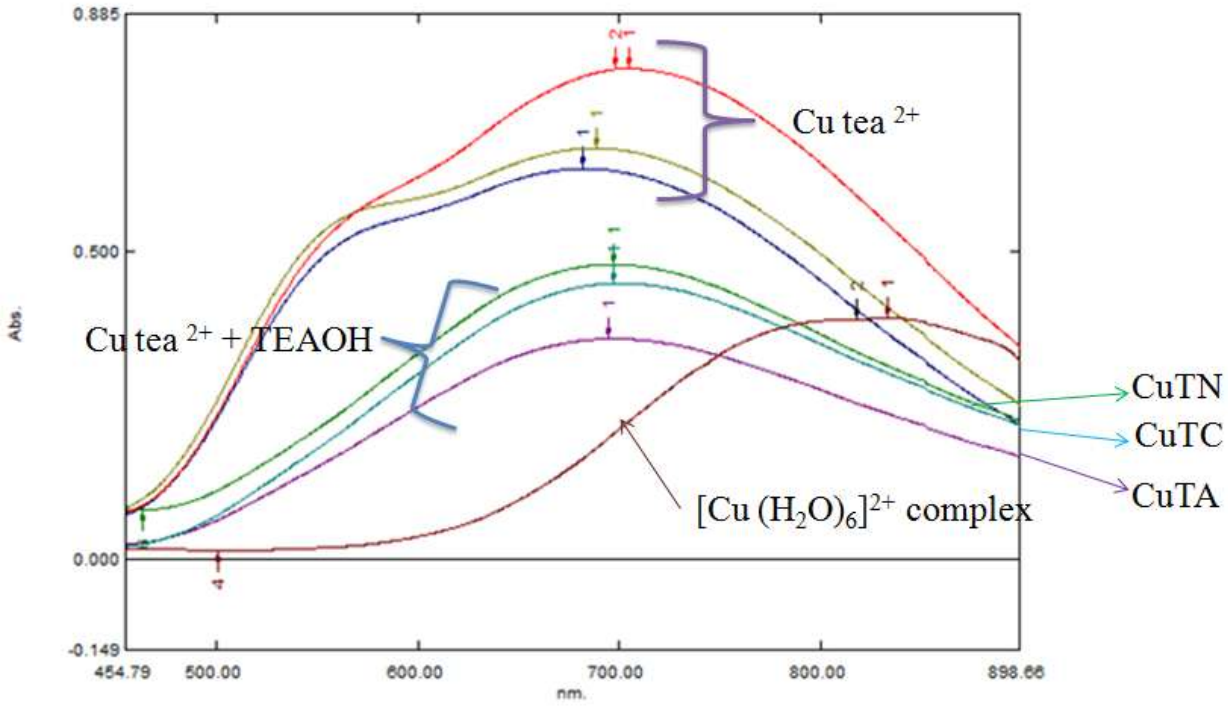

Figure S1. UV Vis spectra of the possible Cu complex formations during the synthesis of CuTUD-1

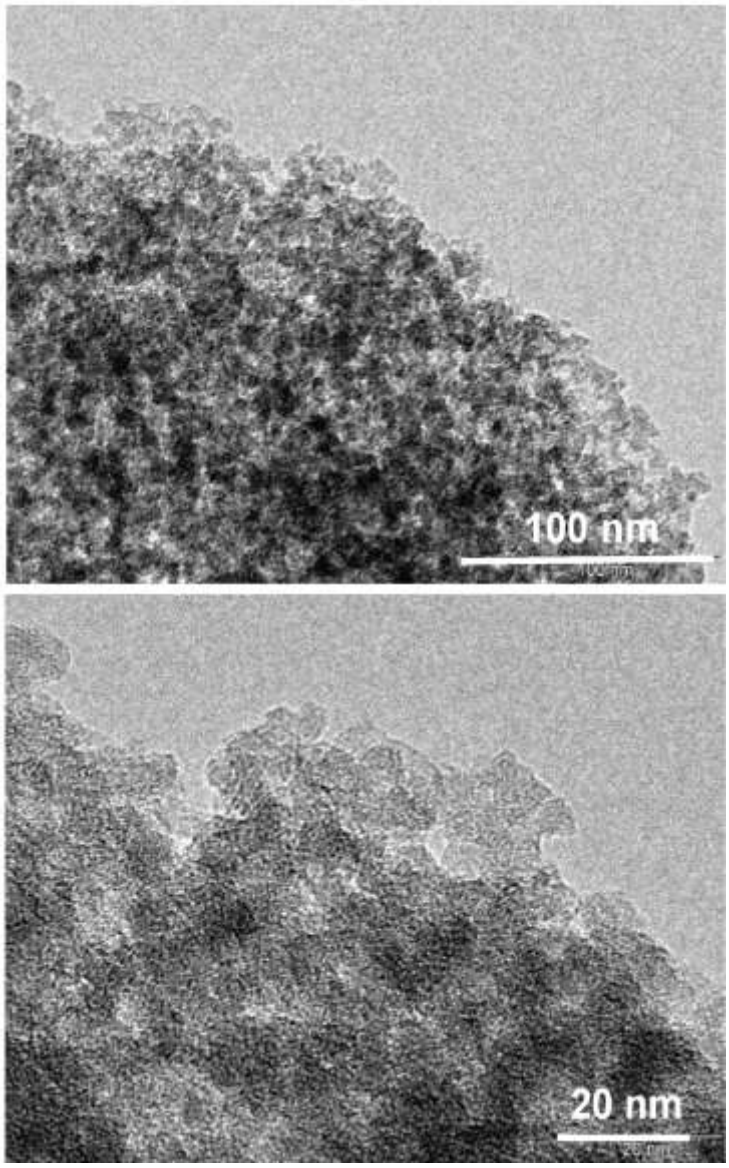

Figure S2. TEM images of CuTN sample

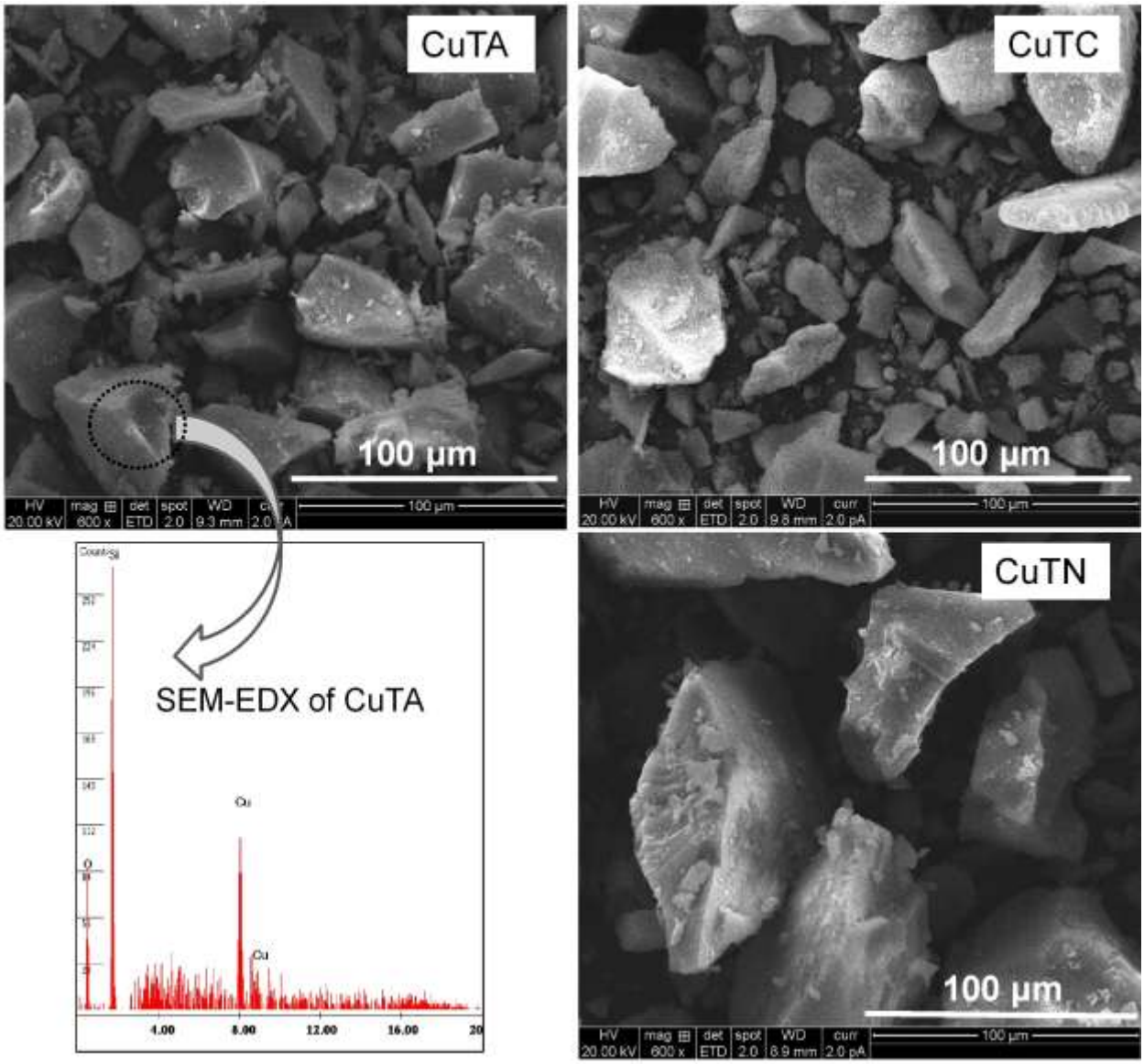

Figure S3. SEM images of CuTA,CuTC and CuTN, EDAX of CuTA sample

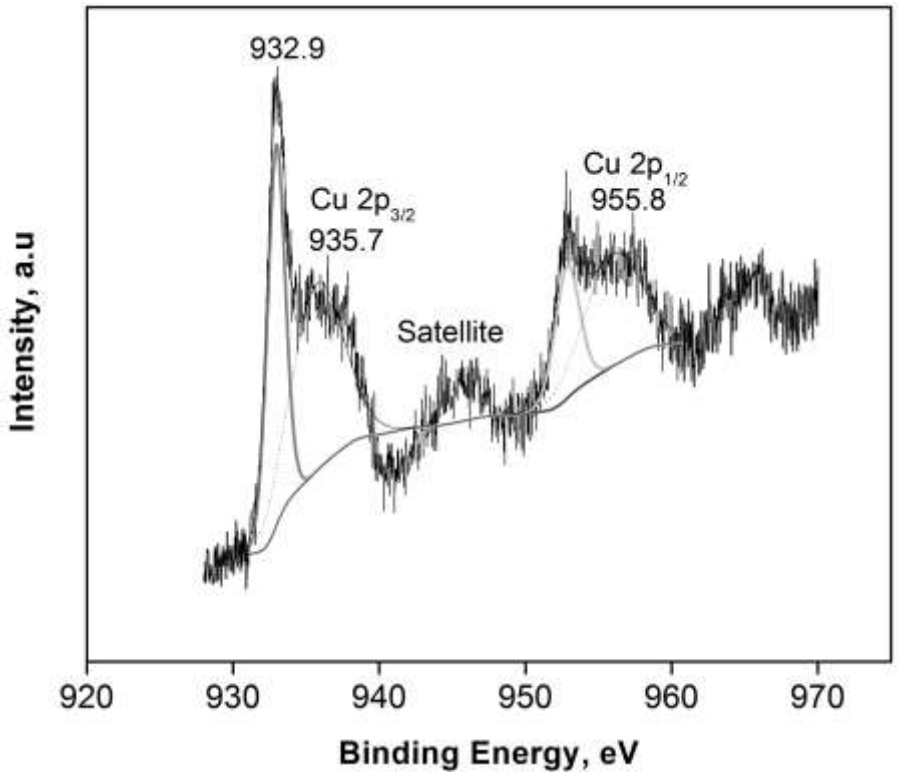

Figure S4. Deconvoluted XPS - Cu 2p core level binding energy spectra of CuTN sample.