

## Supporting information

### Reduction of aromatic nitro compounds catalysed by Biogenic CuO nanoparticles

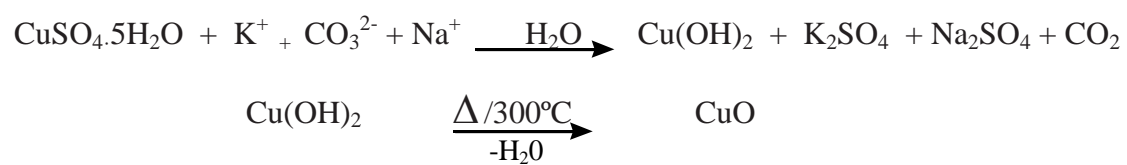
**Chandan Tamuly<sup>a\*</sup>, Indranirekha Saikia<sup>a</sup>, Moushumi Hazarika<sup>a</sup>, and Manash R. Das<sup>b</sup>**

<sup>a</sup> CSIR-North East Institute of Science and Technology. Branch Itanagar Arunachal Pradesh-791110, India

<sup>b</sup> CSIR-North East Institute of Science and Technology. Jorhat, Assam-785006, India

Corresponding author: Telefax: +91360-2244220

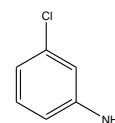
e-mail: c.tamuly@gmail.com



Scheme 1S: Plausible mechanism in synthesis of CuO nanoparticles by using peel of *Musa balbisiana*

## Scheme 2S. Spectroscopic analysis of isolated compounds

### 1) 3-chloroaniline

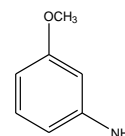


$^1\text{H NMR}$  ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 7.08–7.03 (m, 1 H), 6.80–6.66 (m, 2H), 6.54–6.52 (m, 1H), 3.47 (s, 2H);

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 147.6, 134.8, 130.3, 118.5, 114.9, 113.2

GC-MS ( $m/z$  %): 127.6 ( $\text{M}^+$ ).

### 2) 3-Methoxyaniline

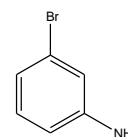


$^1\text{H NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  7.07 (dd,  $J = 8.1$  Hz, 7.8 Hz, 1H); 6.33 (dd,  $J = 8.1$  Hz, 2.4 Hz, 1H); 6.30 (dd,  $J = 7.8$  Hz, 1.8 Hz, 1H); 6.25 (dd,  $J = 2.4$  Hz, 2.4 Hz, 1H); 3.77 (s, 3H); 3.66 (bs, 2H).

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 160.7, 147.2, 130.2, 108.2, 104.4, 101.4, 55.1.

GC-MS( $m/z$ %):123 ( $\text{M}^+$ ).

### 3) 3-Bromoaniline

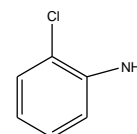


$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.01–6.96 (t, 1H,  $J = 7.6$  Hz), 6.86–6.80 (t, 2H,  $J = 8.5$  Hz), 6.57 (d, 1H,  $J = 7.8$  Hz), 3.67 (br s, 2H).

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 150.4, 131.9, 123.5, 121.3, 115.8, 115.3

GC-MS ( $m/z$ %):172 ( $\text{M}^+$ ).

### 4) 2-Chloro aniline

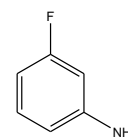


$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.15–7.30(m, 1H), 6.95–7.10(m, 1H), 6.57–6.75(m, 2H), 3.97(bs, 2H)

$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ):  $\delta$  142.6, 128.9, 127.2, 118.6, 118.5, 115.5,

GC-MS( $m/z$ %): 127.6 ( $\text{M}^+$ )

5) 3-Fluoroaniline

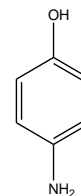


$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$ : 6.98 (t, 1H,  $J = 7.6$  Hz), 6.42-6.80 (t, 2H,  $J = 8.5$  Hz), 6.17 (d, 1H,  $J = 7.8$  Hz), 3.77 (br s, 2H).

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 75 MHz)  $\delta$ : 163.4, 149.9, 131.2, 111.6, 105.8, 104.3

GC-MS( $m/z\%$ ): 111 ( $\text{M}^+$ )

6) 4-Aminophenol



$^1\text{H NMR}$  (300 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  8.95(bs, 1H), 6.31-6.39(m, 4H), 4.00(bs, 2H).

$^{13}\text{C NMR}$  (75 MHz,  $\text{DMSO-d}_6$ ):  $\delta$  148.2, 140.2, 115.4, 115.3.

GC-MS( $m/z\%$ ): 110 ( $\text{M+H}^+$ ).

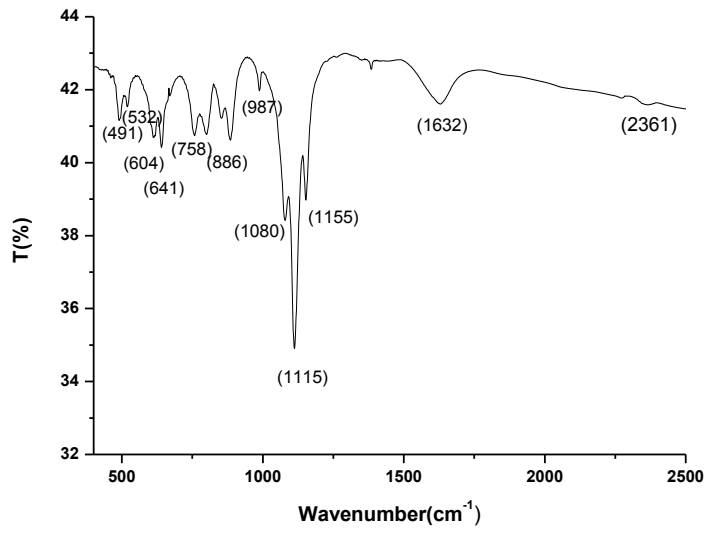


Figure1S: FT-IR spectra of CuO nanoparticles synthesised by *Musa balbisiana*

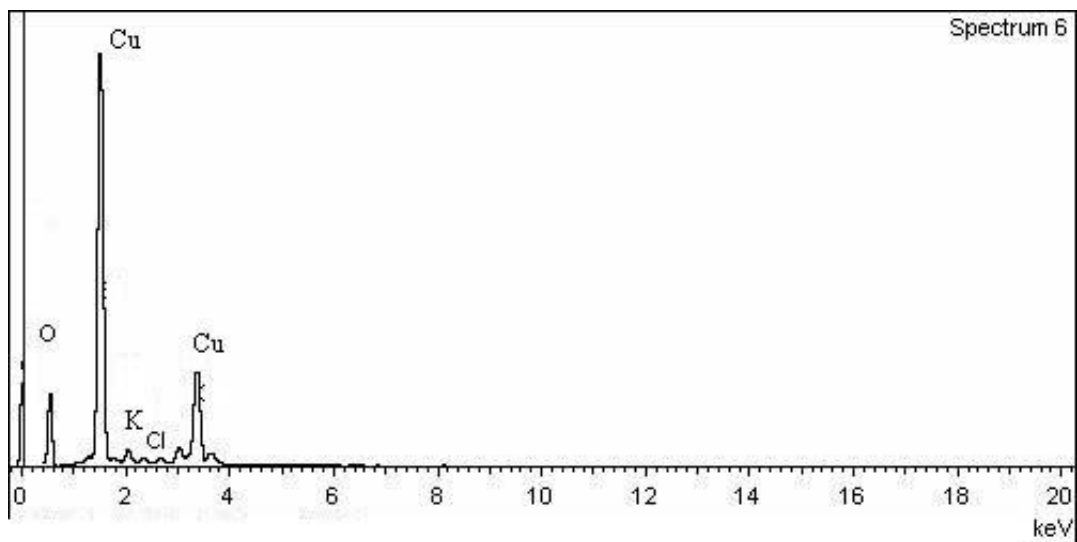


Figure 2S: EDX spectra of CuO nanoparticles.

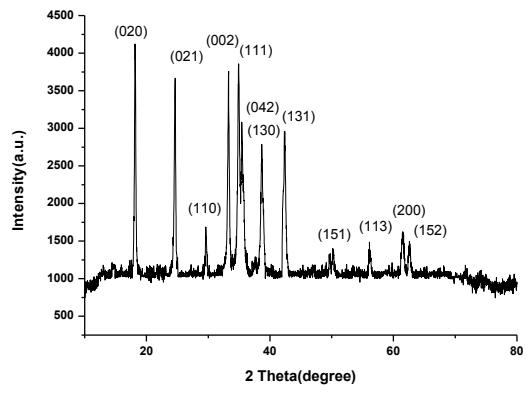


Figure 3S: XRD spectrum of CuO nanoparticles when synthesised by  $K_2CO_3$

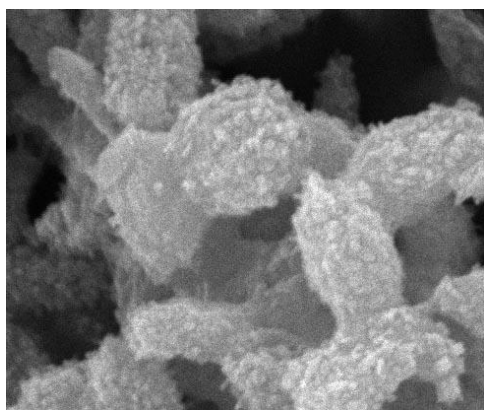


Figure 4S: SEM image of CuO nanoparticles when synthesized by  $K_2CO_3$



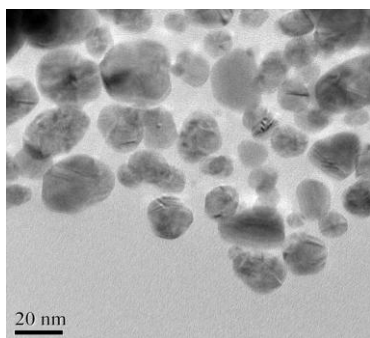


Figure 5S: TEM image of CuO nanoparticles when synthesized by  $K_2CO_3$

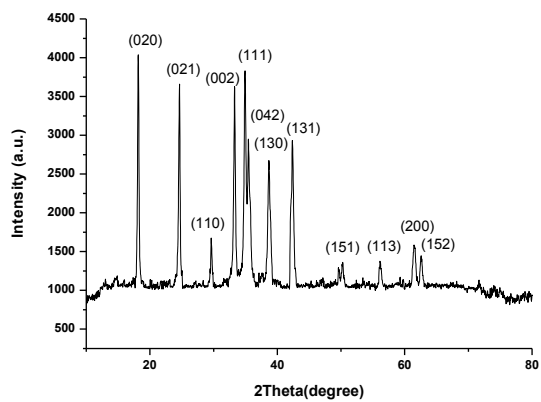


Figure 6S: XRD spectrum of CuO nanoparticles when synthesised by  $\text{Na}_2\text{CO}_3$

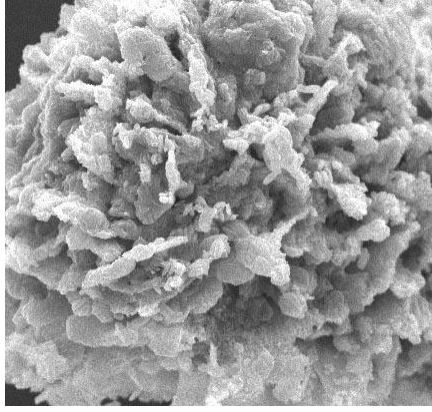


Figure 7S: SEM image of CuO nanoparticles when synthesized by  $\text{Na}_2\text{CO}_3$

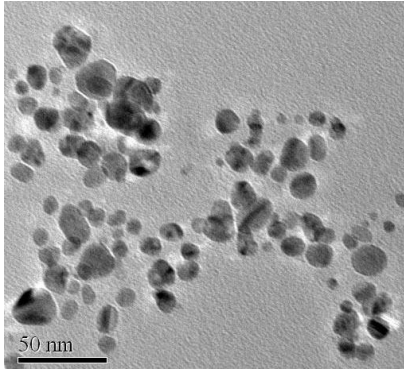


Figure 8S: TEM image of CuO nanoparticles when synthesized by  $\text{Na}_2\text{CO}_3$

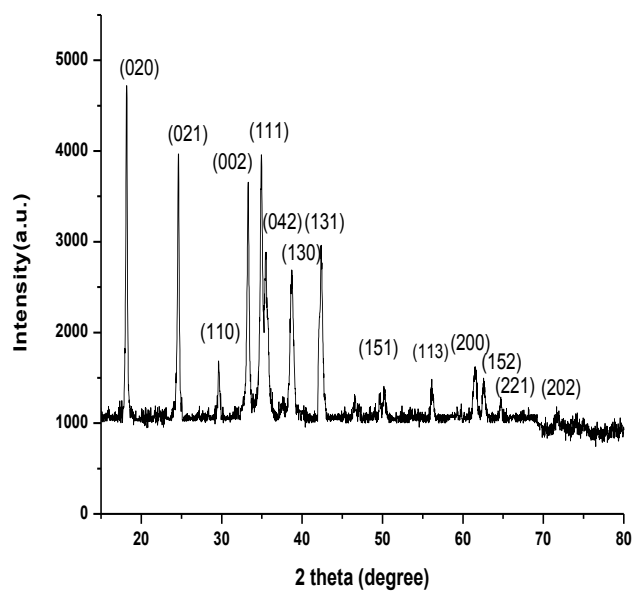


Figure 9S: XRD spectrum of CuO catalyst after 5 recycle

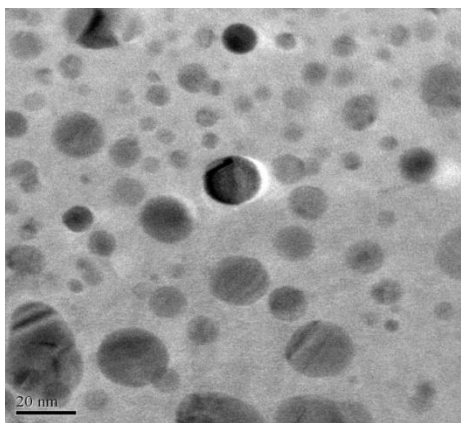


Figure 10S: TEM image after 5 recycle of CuO nanocatalyst

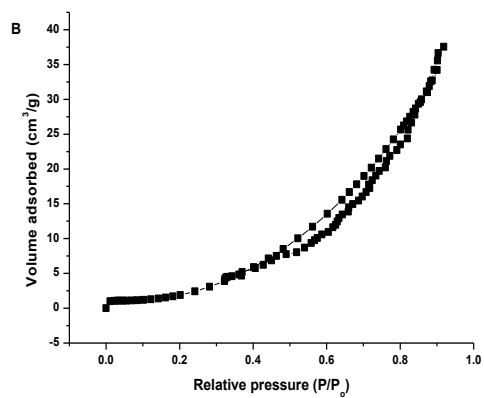
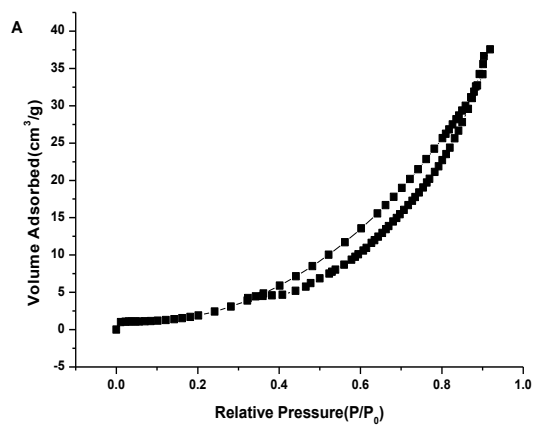


Figure 11S: The stacking pattern of N<sub>2</sub> adsorption desorption curves (A) fresh catalyst (B) after 5<sup>th</sup> cycle

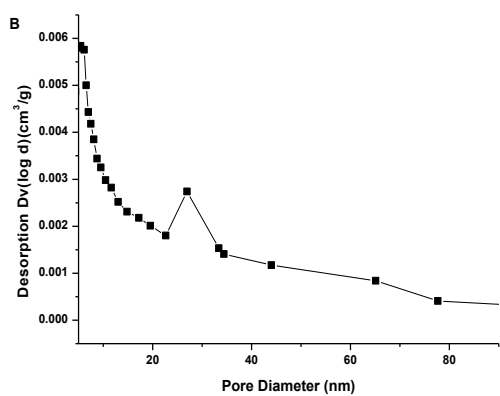
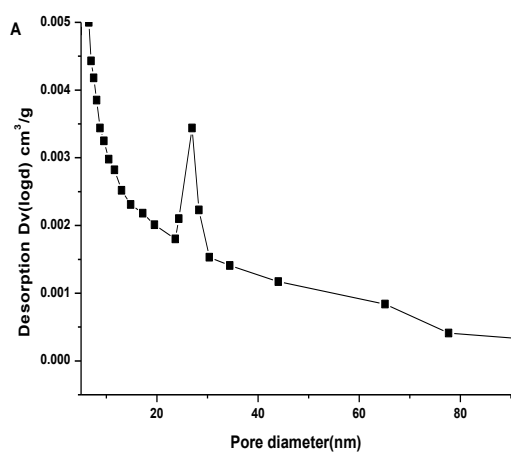


Figure 12S: BJH pore distribution curves of CuO nanoparticles (A) Fresh catalyst (B) After 5<sup>th</sup> cycle



Table 1S: The rate constant of catalytic reduction 4-nitrophenol to 4-aminophenol in presence CuO nanoparticles

Conc. of nanoparticles (mol%)	Rate constant( $\text{min}^{-1}$ )	
	CuO	$R^2$
0.02	0.0781	0.9856
0.04	0.0811	0.9484
0.06	0.0825	0.9723
0.08	0.0850	0.9910
0.10	0.0885	0.9941

Table 2S: CuO catalyzed reduction of aromatic nitro to amino compounds when prepared from commercial  $K_2CO_3$

En-try	Substrate	Product	Time (hr) <sup>a</sup>	Yield (%) <sup>b</sup>	TOF (h <sup>-1</sup> ) <sup>c</sup>
1			1.00	95	950
2			2.00	82	410
3			1.80	80	444
4			2.50	80	320
5			2.30	74	322
6			2.00	75	375

<sup>a</sup> Reactions performed at 30 °C and monitored using TLC until all the aromatic nitro compounds was found to have been consumed.

<sup>b</sup> Isolated yield after column chromatography of the crude product with 2% standard deviation.

<sup>c</sup> TOF: Turn Over frequency