Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2019

Phase Transition in $Cu_{2+x}SnS_{3+y}$ ($0 \leq x \leq 2$; $0 \leq y \leq 1$) Ternary Systems Synthesized with Complexes of Coumarin derived thiocarbamate Motifs: Optical and Morphological Properties

Joseph Adeyemi. Adekoya[1, 2*], Malik Dilshad Khan[2] and Neerish Revaprasadu[2*]

[1]Department of Chemistry, Covenant University, P.M.B. 1023, Ota, Ogun State, Nigeria. [2]Department of Chemistry, University of Zululand, Private Bag X1001, Kwa-Dlangezwa 3886, South Africa.

Supplementary Data

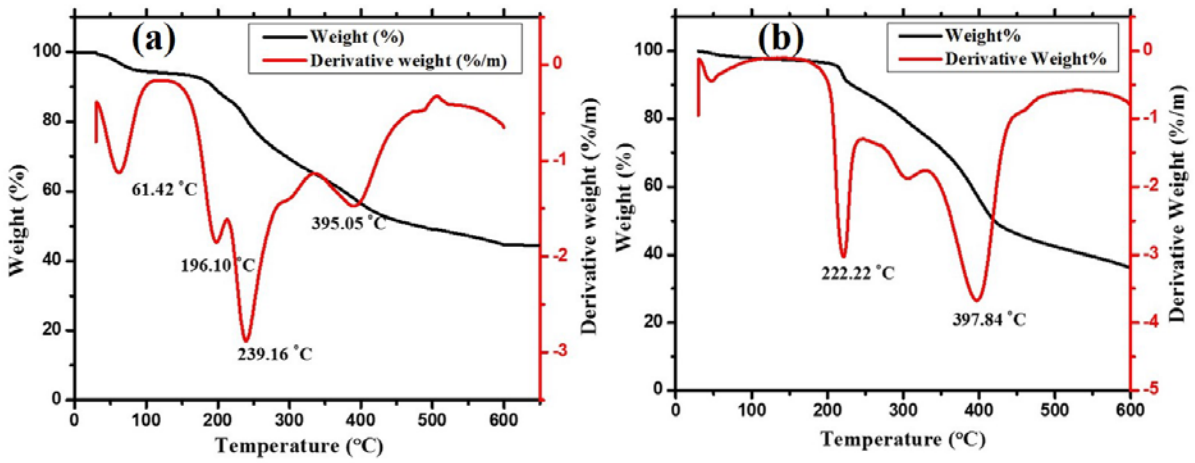

Fig. S1: TGA/ DTA spectrum for (a) Cu(II) and (b) Sn(II) complex respectively.

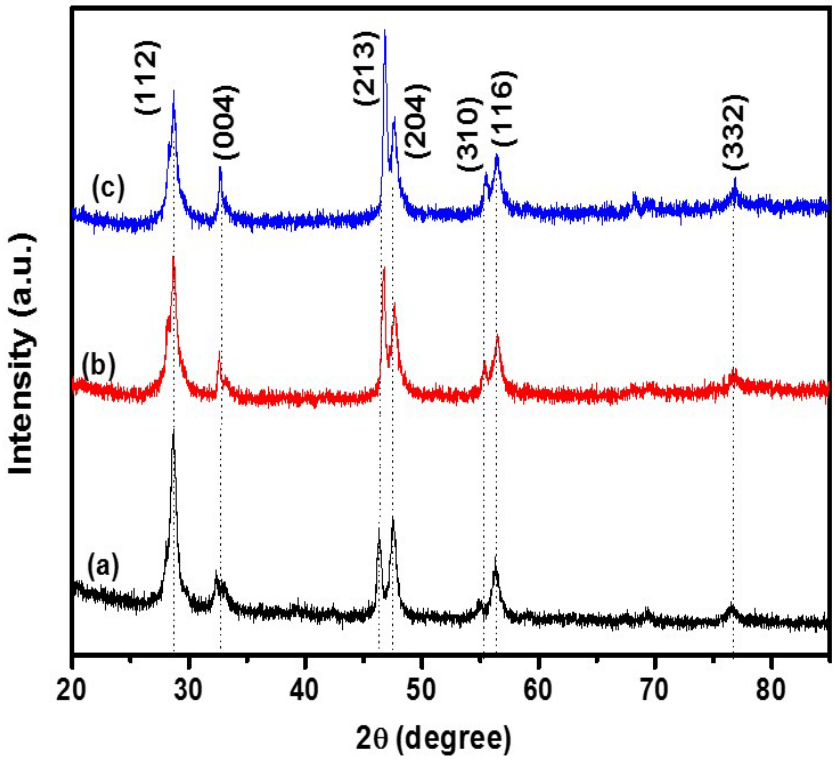

Fig. S2: p-XRD pattern of tetragonal CTS NPs obtained at 200 °C for (a) 2.1:1 (b) 1.7:1 (c) 2.2:1 of Cu/Sn ratio precursors (Heat up).

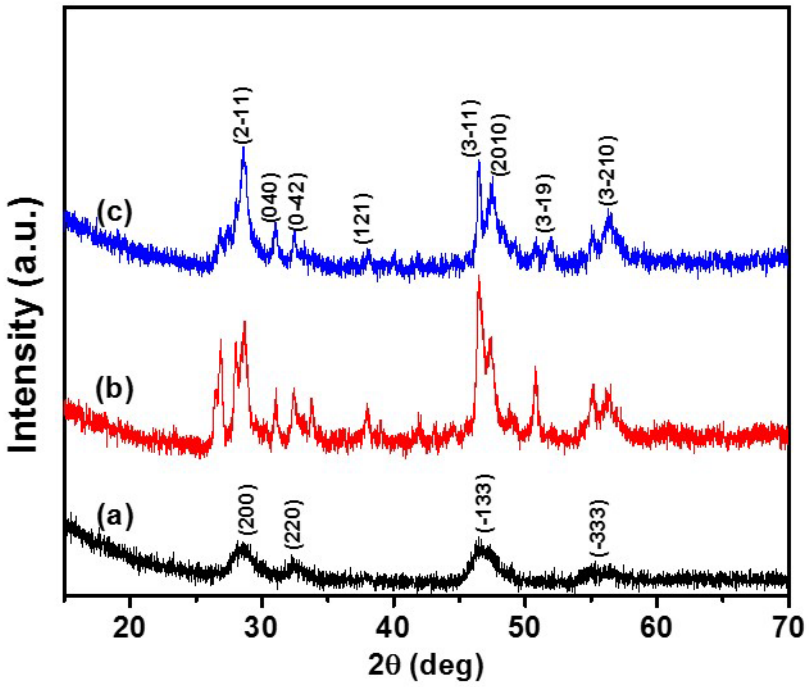

Fig. S3: p-XRD patterns of Mohite, Syn anorthic CTS phase obtained by hot injection of (a) monoclinic CTS phase by injection of 2.0 mL OLA/precursors in 6.0 mL DT at 200 °C, (b) 2.0 mL OLA/precursors in 6.0 mL DT at 250 °C and (c) 2.0 mL OLA/precursors in 6.0 mL OLA at 200 °C.

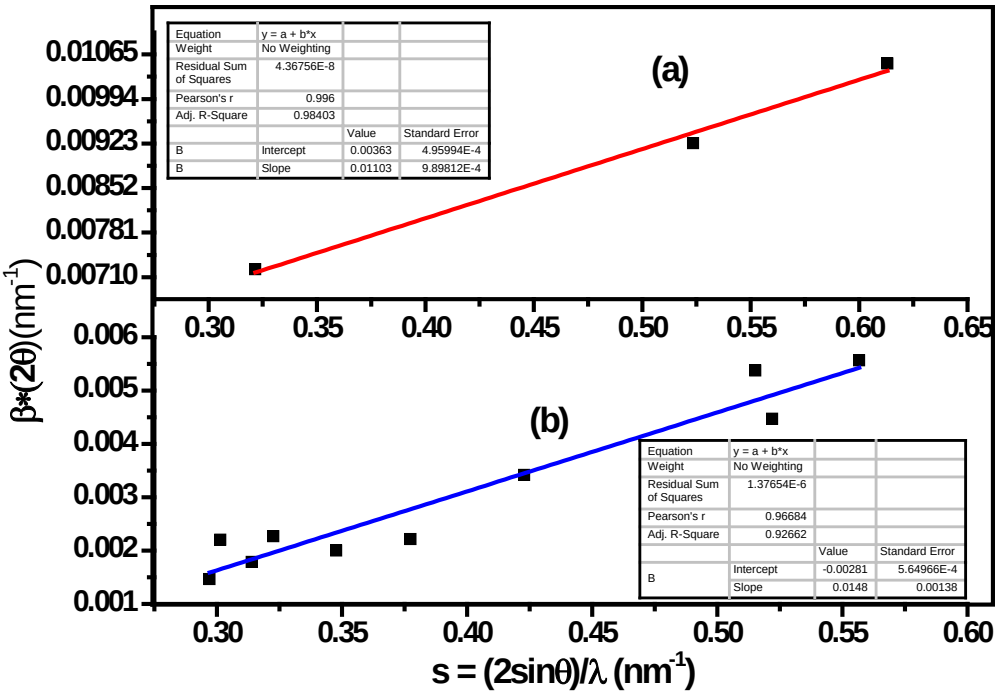

Fig. S4: Average size of coherent scattering regions, CSR estimated from broadening of non-overlapping diffractions for (a) Tetragonal (b) Orthorhombic CTS phase using selected 2θ diffraction angles in Fig. 1b and Fig. S3(c) respectively.

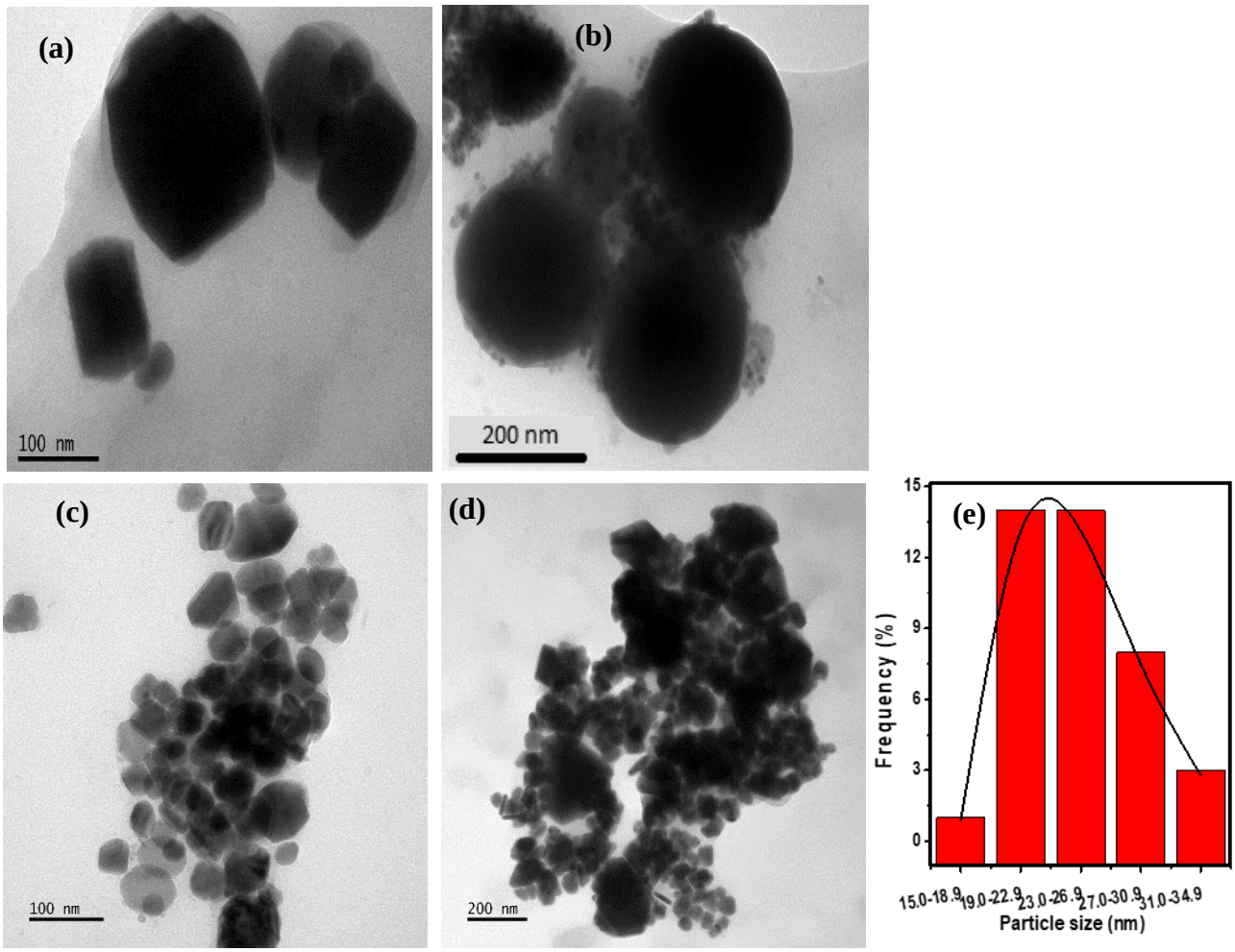

Fig. S5: TEM micrographs of (a) CTS orthorhombic nanodiscs in OLA/DT at 250 °C (b) CTS nanosphere in OLA/OLA at 200 °C (c, d) CTS nanohexagons obtained by hot injection method at 200 °C and (e) its particle size histogram.

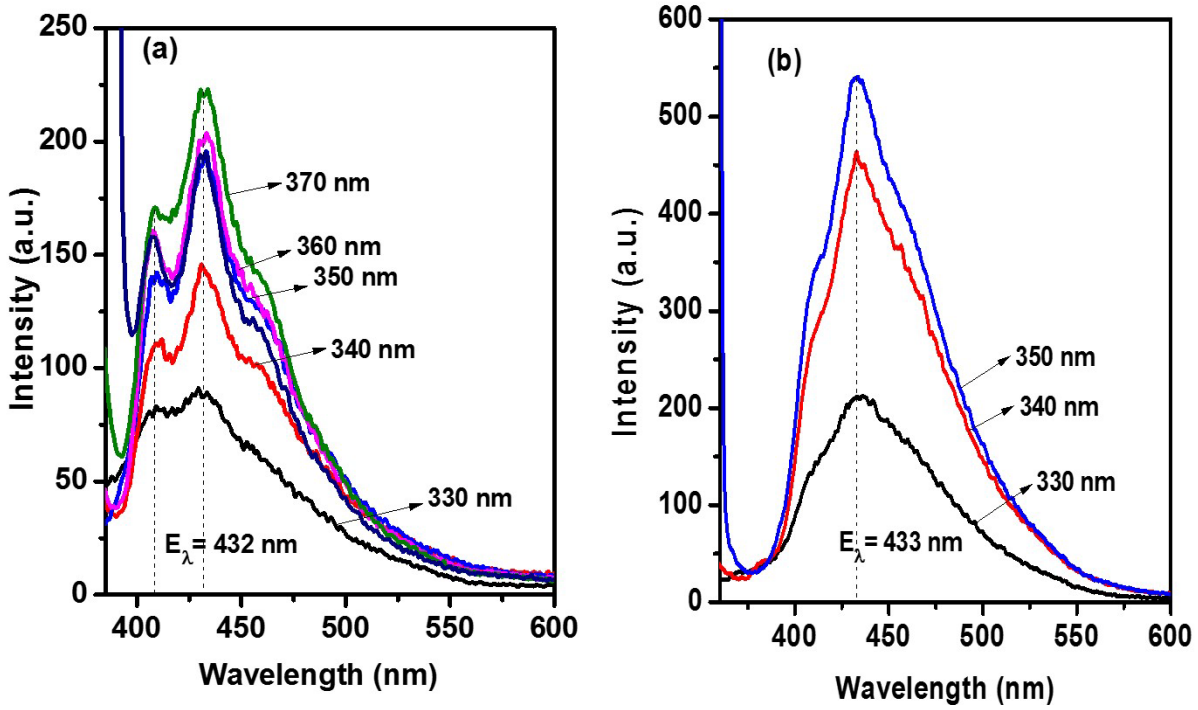

Fig. S6: Optical emission spectra of CTS NPs obtained by hot injection in DT at (a) 250 °C (b) 200 °C.

Table S1: Structural parameters obtained from Rietveld refinements of the p-XRD pattern and the stoichiometric of atomic concentrations and weight percentage for the Cu_2SnS_3 Mohite Syn Monoclinic phase.

	Mohite Syn Monoclinic: Cu_2SnS_3			
	Space Group			**C1c1**
Cell parameters	a (Å)	6.8777(1)Å		
	b (Å)	11.4848(2)Å		
	c (Å)	6.70099(1)Å		
	β	110.787(3)°		
Atomic positions		**X**	**Y**	**Z**
	Cu (1)	-0.0133	0.2563	0.4984
	Cu (2)	-0.0253	0.4125	-0.0181
	S (3)	0.3545	0.4222	0.1123
	S (4)	0.3589	0.2379	0.6179
	S (5)	0.3779	0.0905	0.1185
	Sn (6)	0	0.0898	0
Weight fractions (in %)	94.084(4)			
Final weighted average Bragg R-factor	25.0			
Final reduced chi^2	9.5			

Table S2: Chemical composition of final CTS NPs

Chemical composition along with composition ratio (at%)				
Sample	Cu	Sn	S	Cu/Sn
CTS#6	33.86	17.76	48.38	1.91