

Synthesis of Shape and Size Controlled Copper Indium Diselenide (CuInSe₂) via Extrusion of Selenium from 1, 2, 3-Selenadiazole

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Supplementary Information

Table S1 Calculated and measured particle size, band gap and lattice strain of as-synthesized ClSe NPs at various reaction conditions.

Sample	Average crystallite size from XRD (nm)	Particle size from Williamson-Hall plot (nm)	Particle size from particle size analyzer (nm)	Band gap (eV)	Lattice strain from Williamson-Hall plot (Unit x10 ⁻³)
A)		Effect of temperature			
(a) @175°C	20	26	12	1.4	0.87
(b) @195°C	28	37	15	1.1	1.2
(c) @200°C	28	36	10	1.2	0.74
(d) @230°C	8	8.6	7	1.2	-0.47
(e) @240°C	26	31	13	1.1	0.66
(f) @250°C	29	35	24	1.2	0.65
B)		Effect of amount of OA			
(g) 5 ml OLA	26	35	24	1.1	1.3
(h) 10 ml OLA	22	22	11	1.2	-0.9
(i) 15 ml OLA	15	17	9	1.3	-1.5
C)		Effect of different capping agents and solvent			
(j) OLA+ DPE	24	26	35	1.4	-2.7
(k) OLA +DDA +OD	20	27	11	1.7	-0.5
(l) MPA	23	24	25	1.3	0.24

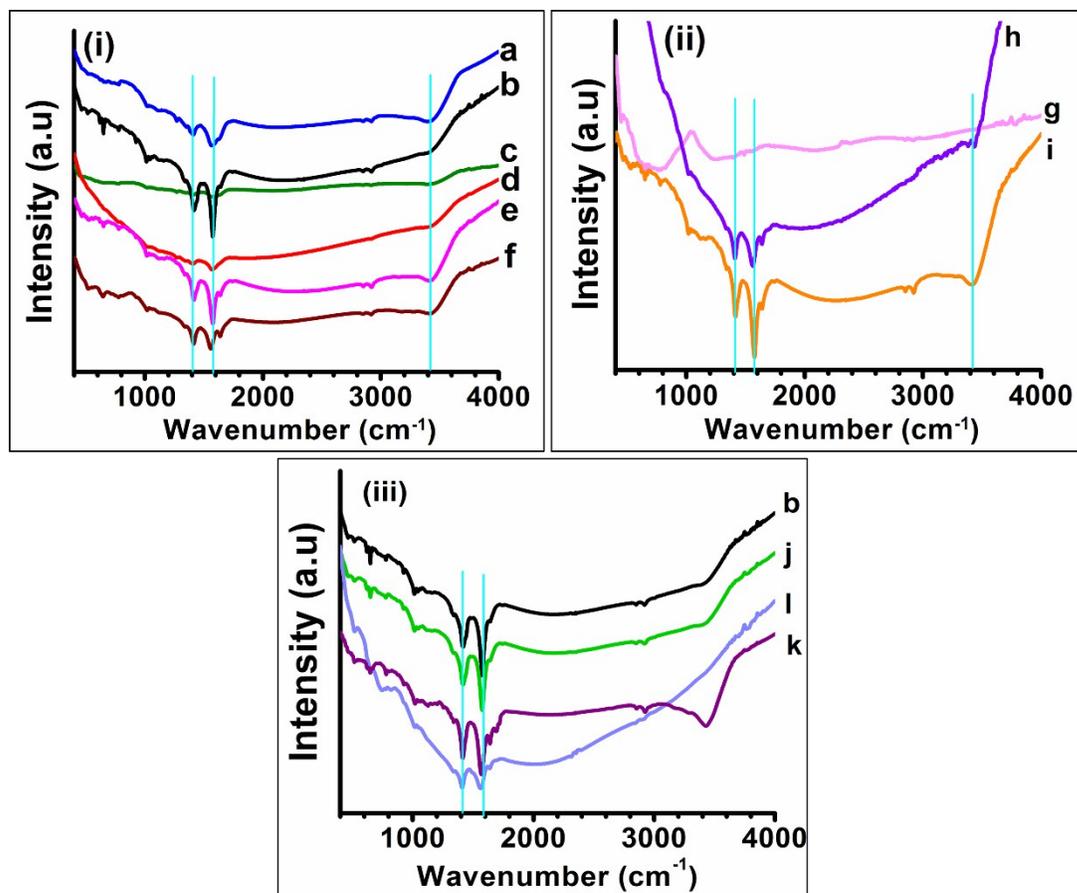


Fig. S1. FTIR of CISE NPs (i) synthesized at 175° (a), 195° (b), 200° (c), 230° (d), 240° (e) and 250°C (f); (ii) synthesized using 5 ml (g) OLA, 10 ml OLA (h) and 15 ml OLA (i), (iii) synthesized using OLA+ DPE (j), OLA +DDA +OD (k) and MPA (l).

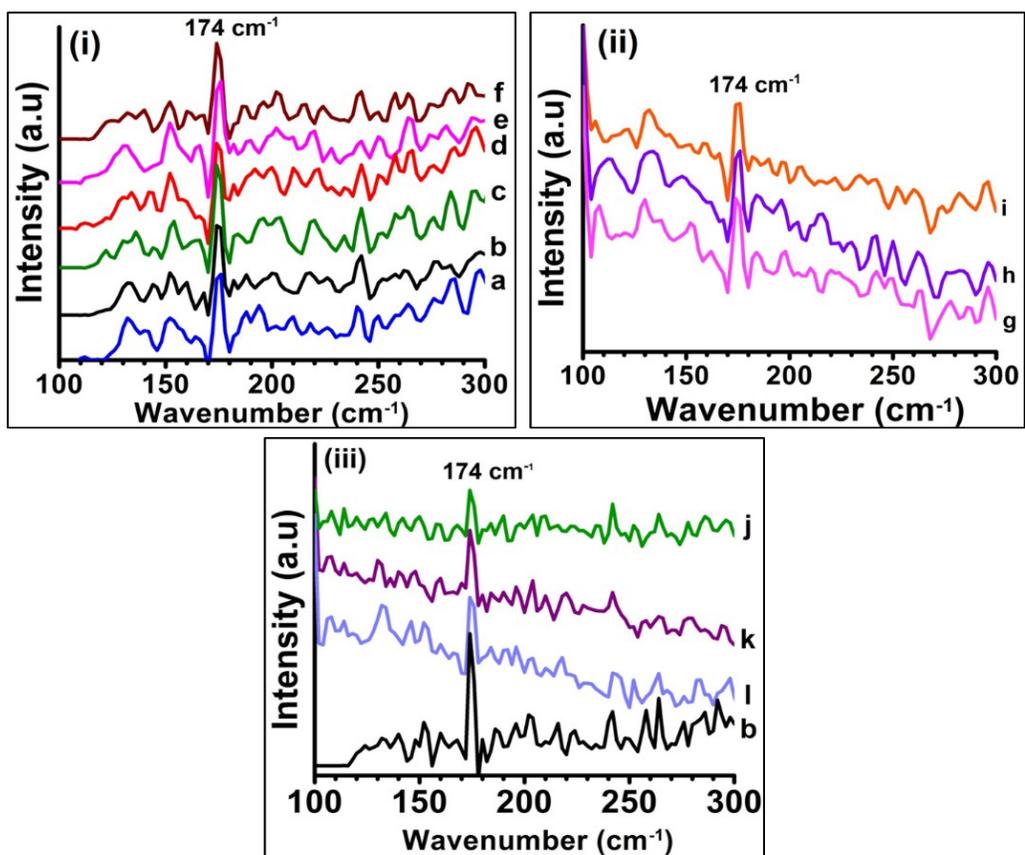


Fig. S2. Raman scattering of ClSe NPs (i) synthesized at (a) 175°, (b) 195°, (c) 200°, (d) 230°, (e) 240° and (f) 250°C (ii) synthesized using (g) 5 ml OLA, (h) 10 ml OLA, (i) 15 ml OLA, (iii) synthesized using (j) OLA and DPE, (k) OLA, DDA, OD and (l) MPA.

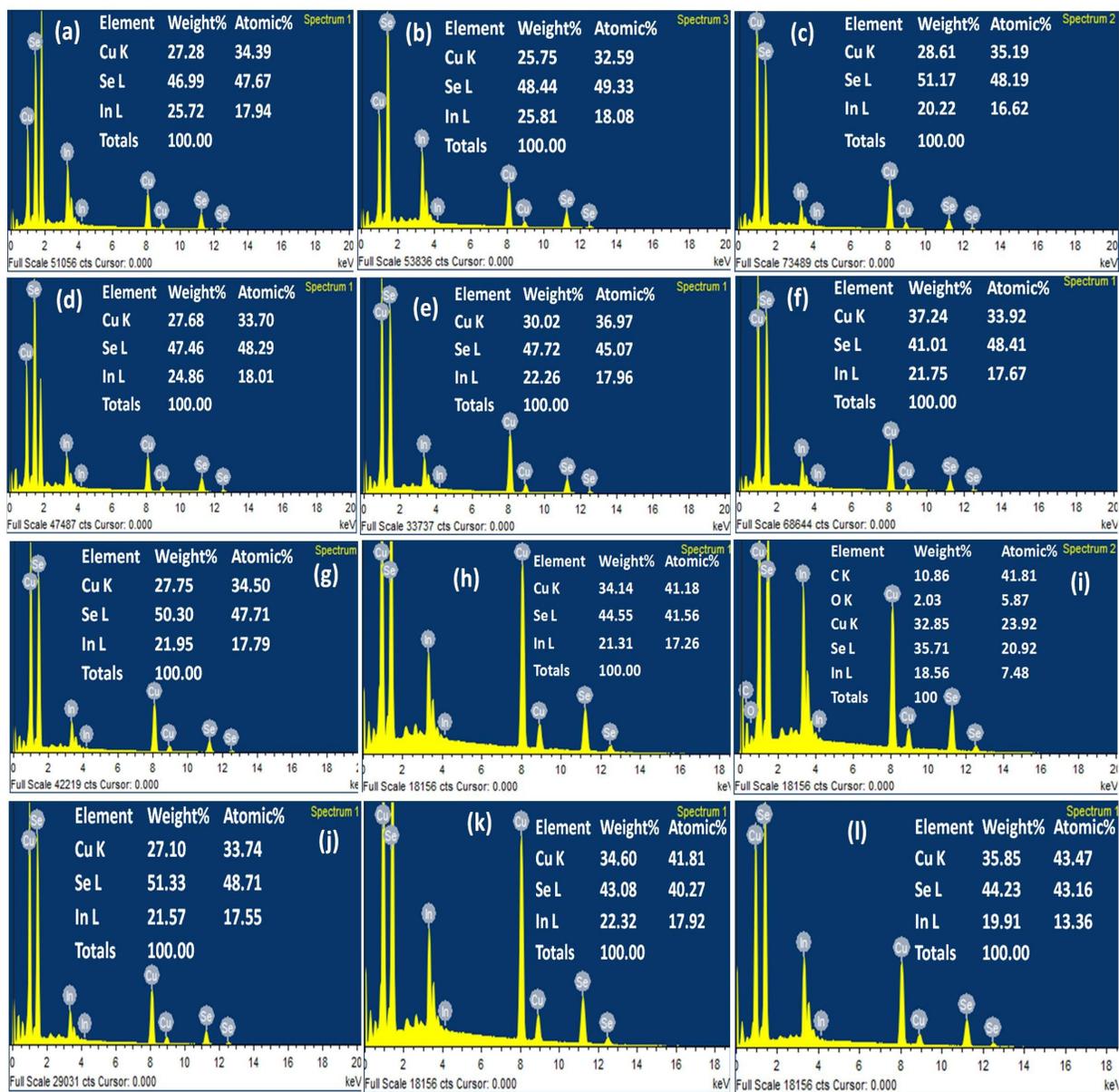


Fig. S3. EDAX analysis of CISE NPs synthesized at various temperatures (a-f), using different concentration of OLA (g-i) and various capping agents (j-l).

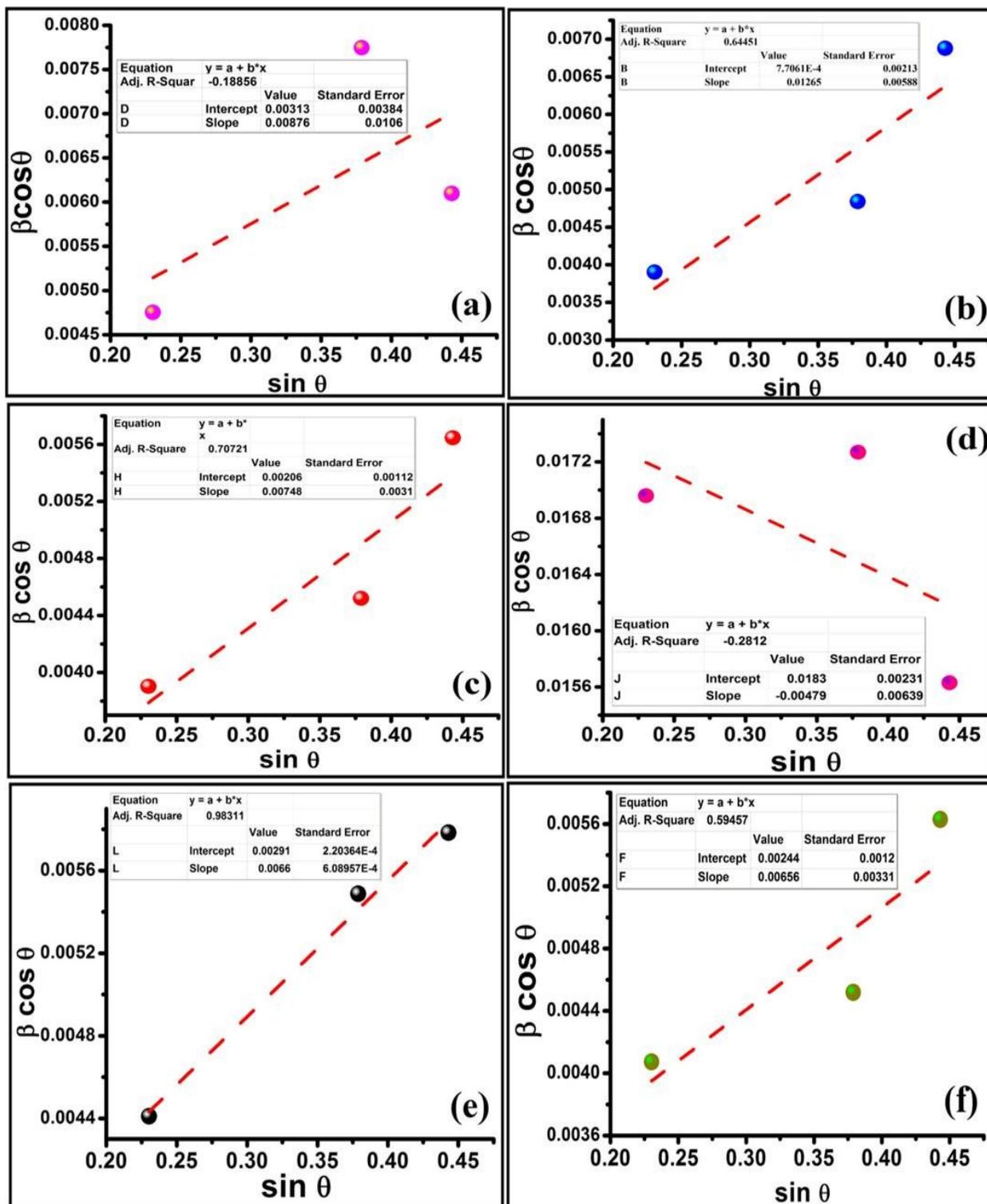


Fig. S4. The W-H analysis assuming UDM of CISE NPs synthesized at various temperatures.

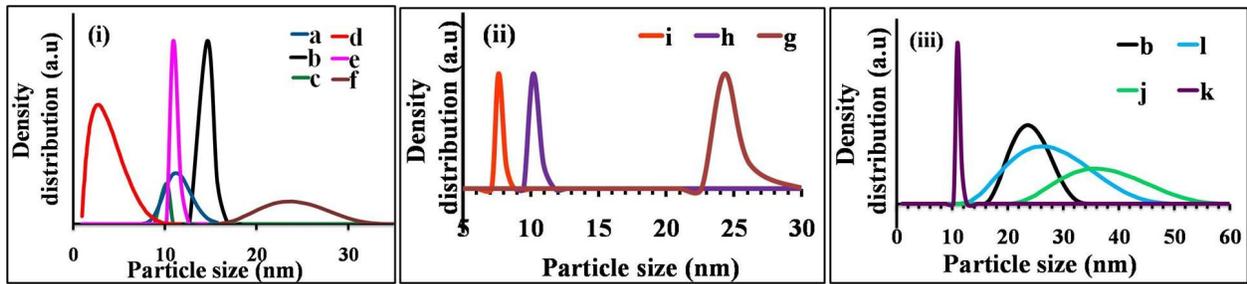


Fig. S5. Particle size analyses of as-synthesized CuSe NPs at (i) at various temperature, (ii) using various amount of capping agent and (iii) different capping agents

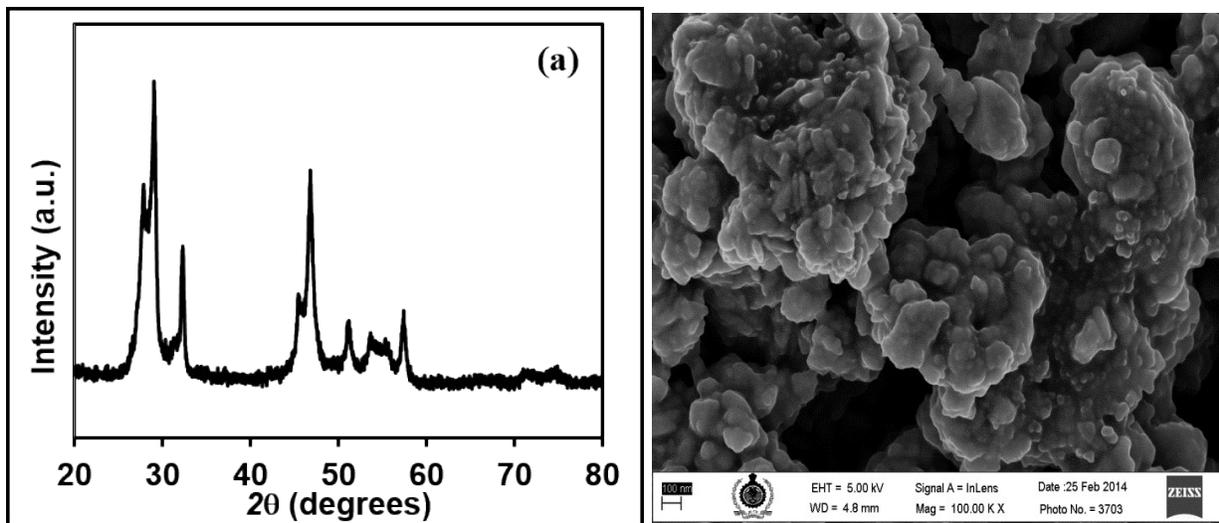


Fig. S6. a) XRD and b) SEM image of CuSe NPs synthesized at 155°C.

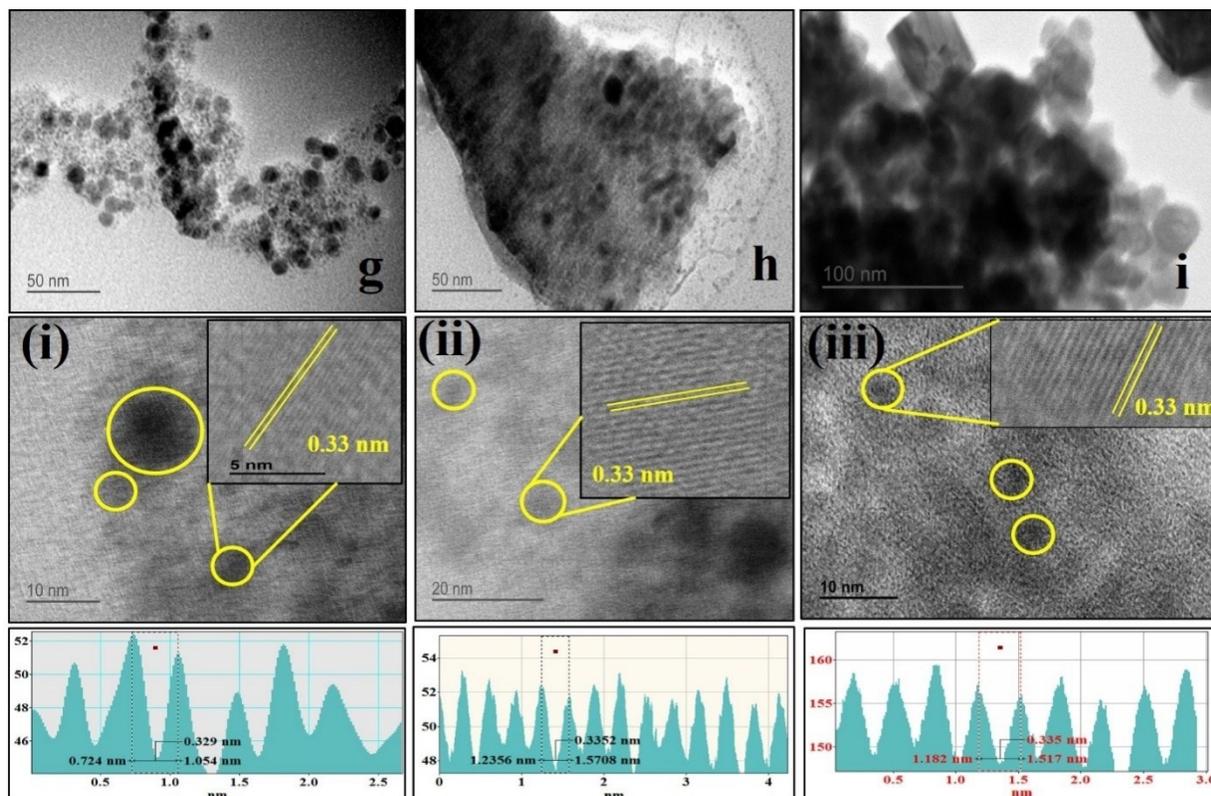


Fig. S7. TEM images of ClSe NPs synthesized using 5 ml (g), 10ml (h) and 15ml (i) OLA as capping agent. Figure (i), (ii) and (iii) are HRTEM of (g), (h), (i) respectively. Inset shows lattice fringes of ClSe NPs.

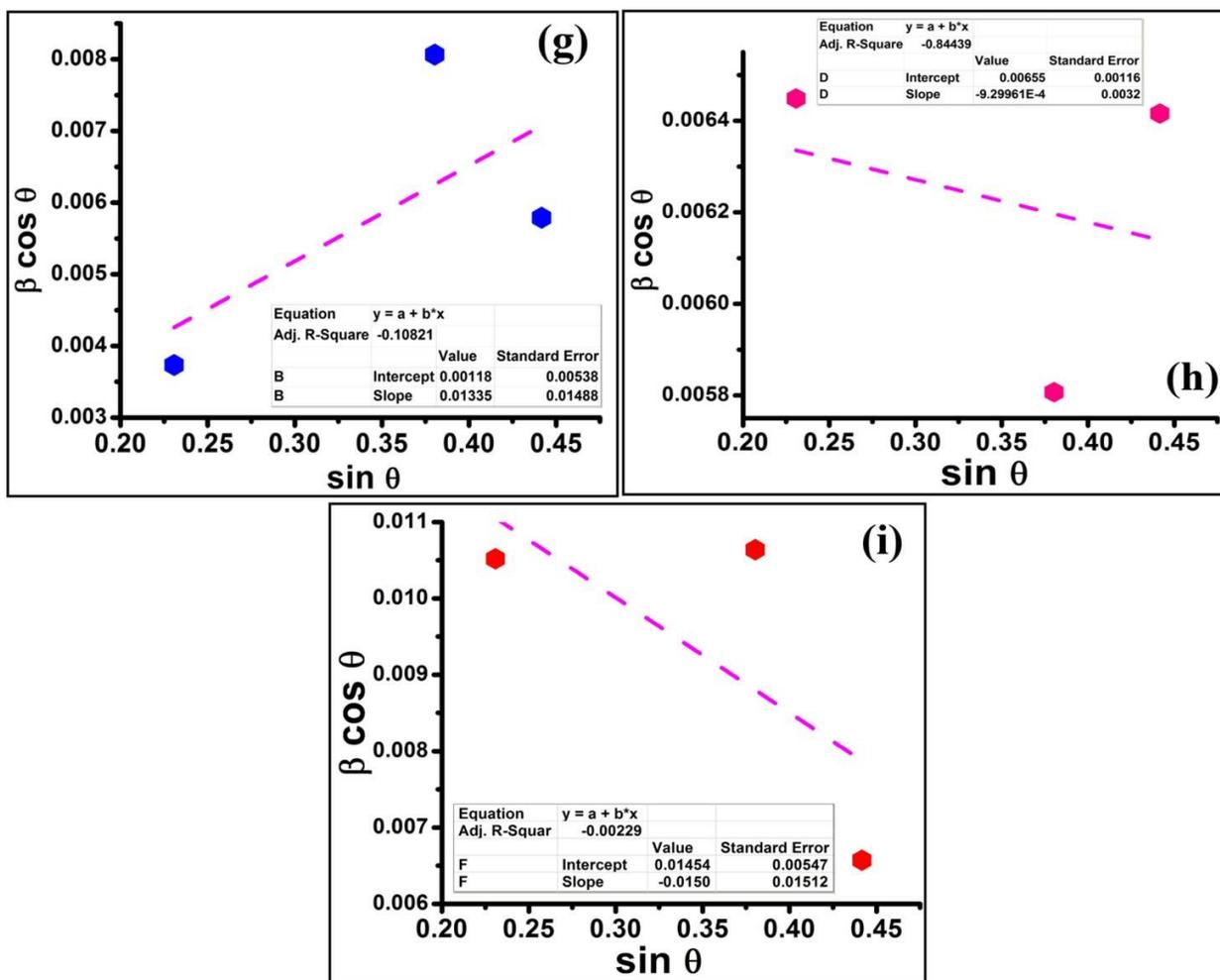


Fig. S8. The W-H analysis assuming UDM of CISE NPs synthesized using different concentration of OLA.

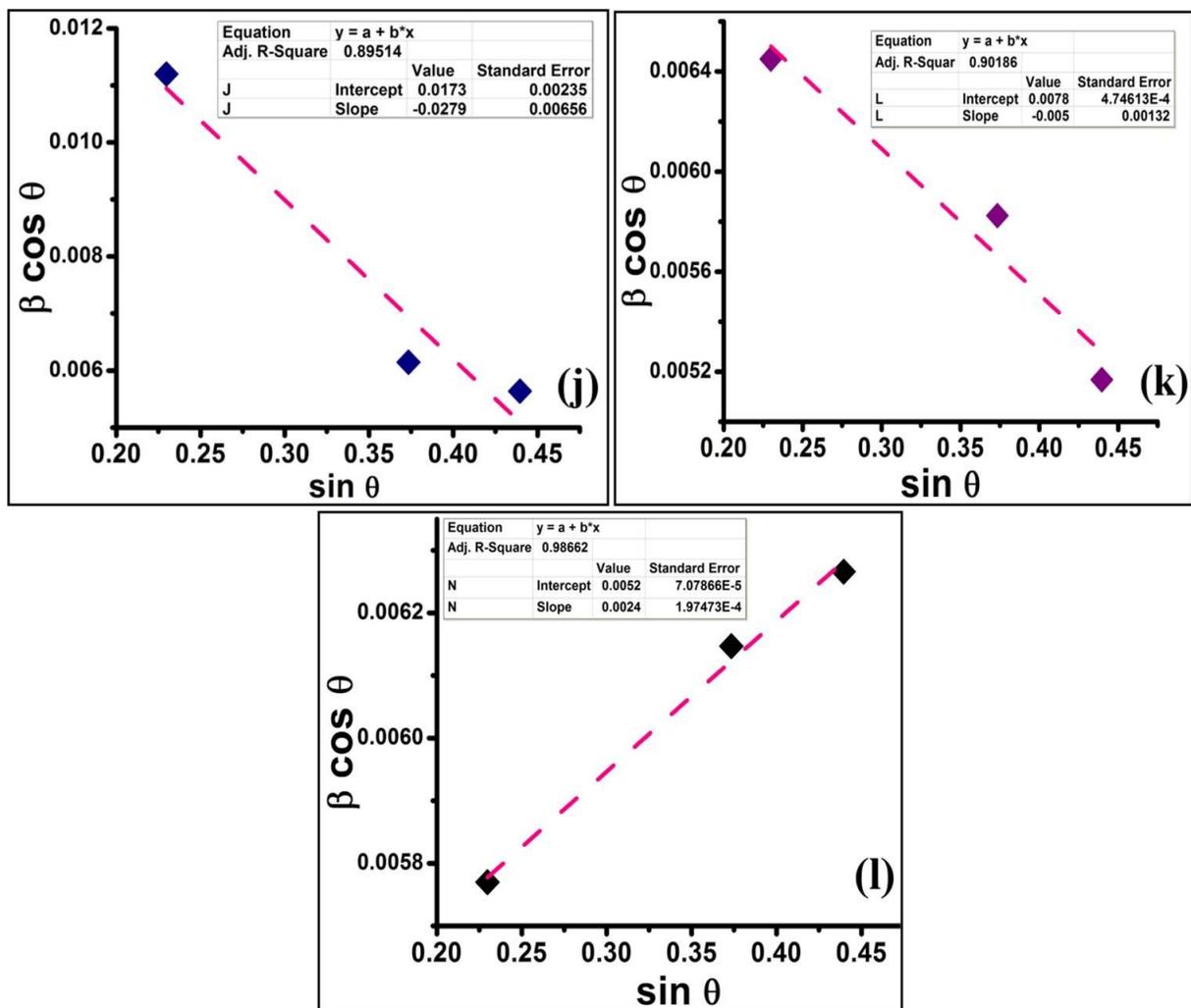


Fig. S9. The W-H analysis assuming UDM of CISE NPs synthesized using combination of capping agents.

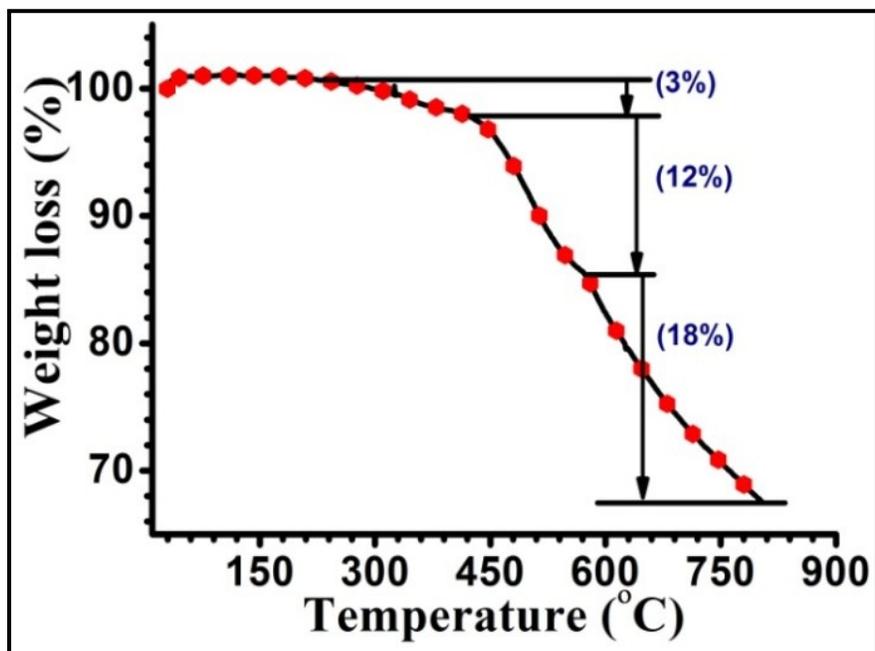


Fig. S10. TGA of oleic acid capped CdSe NPs