

Synthesis and Structure of [(Ph₃P)₂Cu(μ -SeCH₂Ph)₂In(SeCH₂Ph)₂] as Single-Source Precursor for the Preparation of CuInSe₂ Nanomaterials

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Intensity data for [(PPh₃)₂CuIn(SeCH₂C₆H₅)₄] was collected on a SuperNova CCD diffractometer. The crystals were kept at 293 ± 1 K during data collection. The structures were solved using Olex2 [1]. Refinement was done using structure solution program by Direct Method ShelXL [2] refinement package using Least Squares minimisation. The non-hydrogen atoms were refined anisotropically and fitted with hydrogen atoms in their calculated positions. The molecular structures were drawn using ORTEP. Crystallographic and structural determination data are given in Table 1.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J.A.K. Howard, H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.
2. SHELXS G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112-122.

Table S1: Crystallographic and structure refinement data for [(PPh₃)₂CuIn(SeCH₂C₆H₅)₄]:

Compounds	[(PPh ₃) ₂ CuIn(SeCH ₂ C ₆ H ₅) ₄]
Chemical Formula	C ₆₄ H ₅₈ CuInP ₂ Se ₄
Formula weight	1383.24
Crystal Size (mm ³)	0.275 × 0.148 × 0.108
Diffractometer	SuperNova CCD
T/K	293
λ/Å	CuKα (λ = 1.54184)
Crystal system	Monoclinic
Space group	C2/c
a/Å	22.6988(9)
b/Å	13.1304(4)
c/Å	21.1832(10)
α/°	90
β/°	110.171(5)
γ/°	90
V/Å ³	5926.3(4)
ρ _{calc} /g cm ⁻³	1.550
Z	4
μ/mm ⁻¹	7.156
Reflection collected	5251
Data/restraints/parameters	5291/0/296
Final R ₁ , wR ₂ indices	R ₁ = 0.0684, wR ₂ = 0.1727
R ₁ , wR ₂ (all data)	R ₁ = 0.1175, wR ₂ = 0.2523
Largest diff. peak & hole [eÅ ⁻³]	1.02 and -1.25

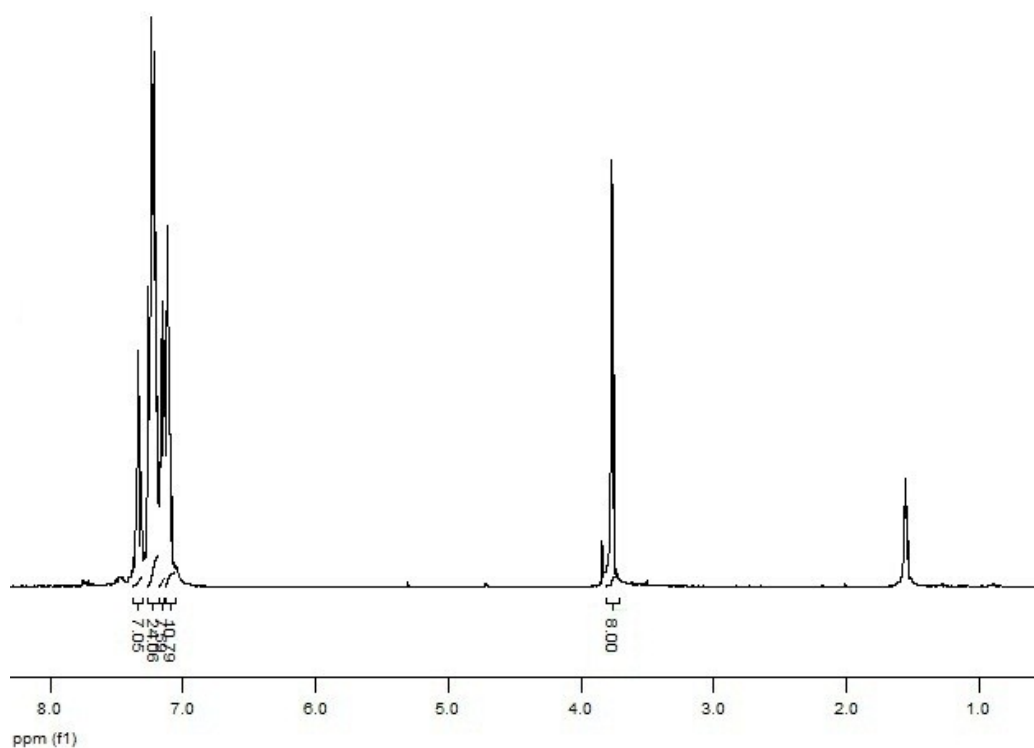


Figure S1: ^1H NMR spectra (500 MHz, CDCl_3) of $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$.

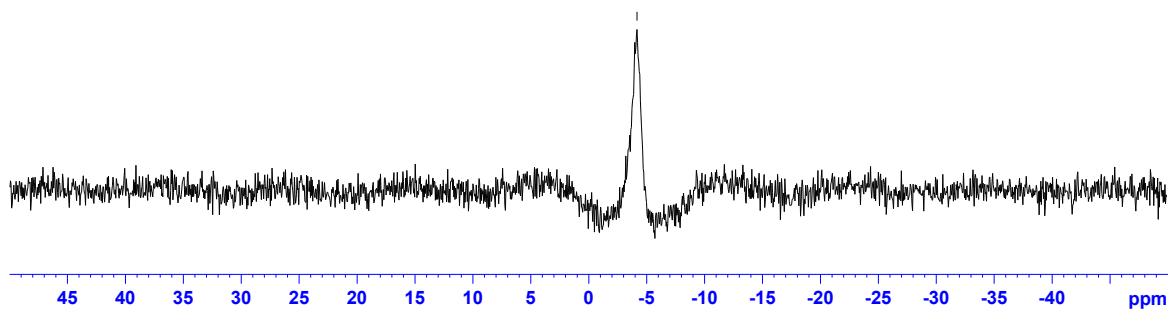


Figure S2: $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (242 MHz, CDCl_3) of $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$.

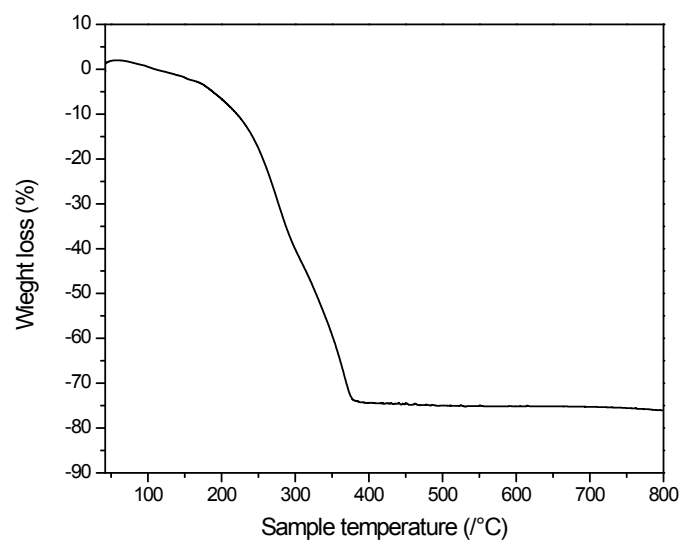


Figure S3: TG curve for $[(PPh_3)_2CuIn(SeCH_2C_6H_5)_4]$

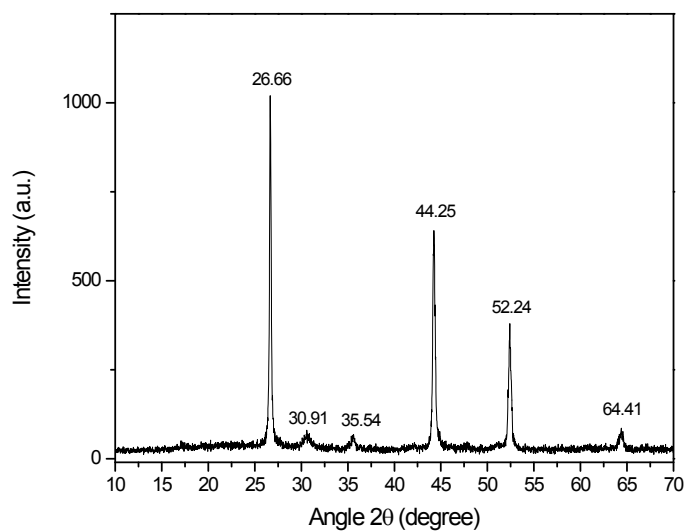


Figure S4: Powder XRD of $CuInSe_2$ obtained from $[(PPh_3)_2CuIn(SeCH_2C_6H_5)_4]$ on thermolysis in a furnace at 400 °C for 2h in argon atmosphere.

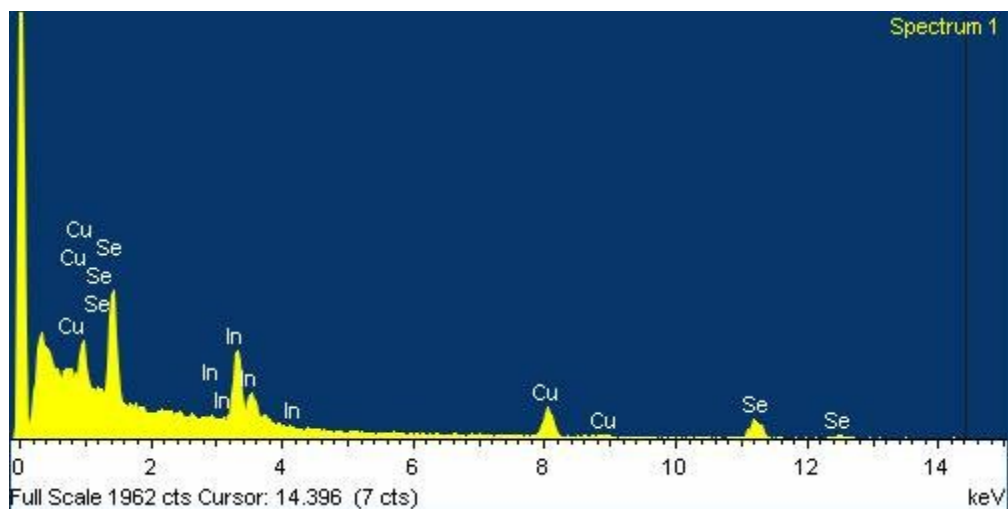


Figure S5: EDX spectrum of CuInSe_2 obtained from furnace heating of $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $400\text{ }^\circ\text{C}$ for 2h.

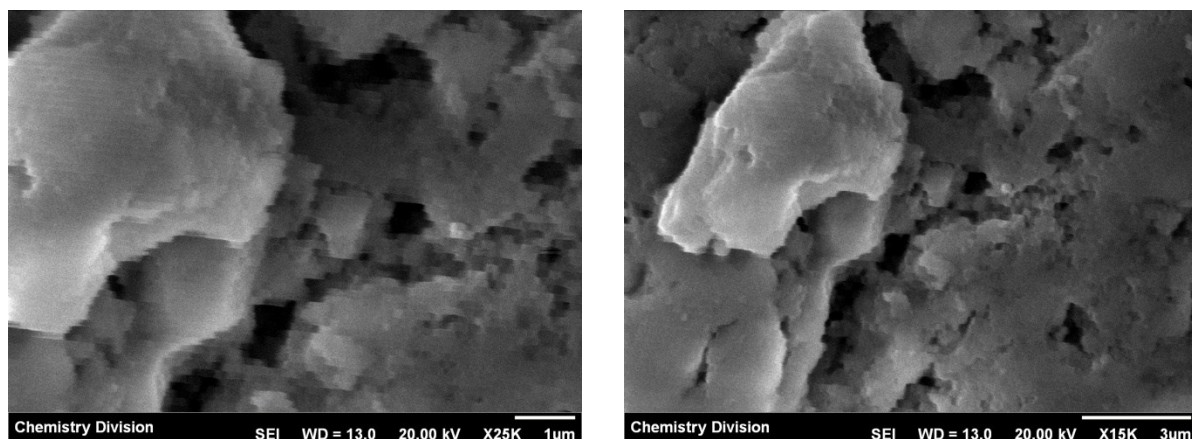


Figure S6: SEM images with different magnifications of CuInSe_2 obtained from furnace heating of $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $400\text{ }^\circ\text{C}$ for 2h.

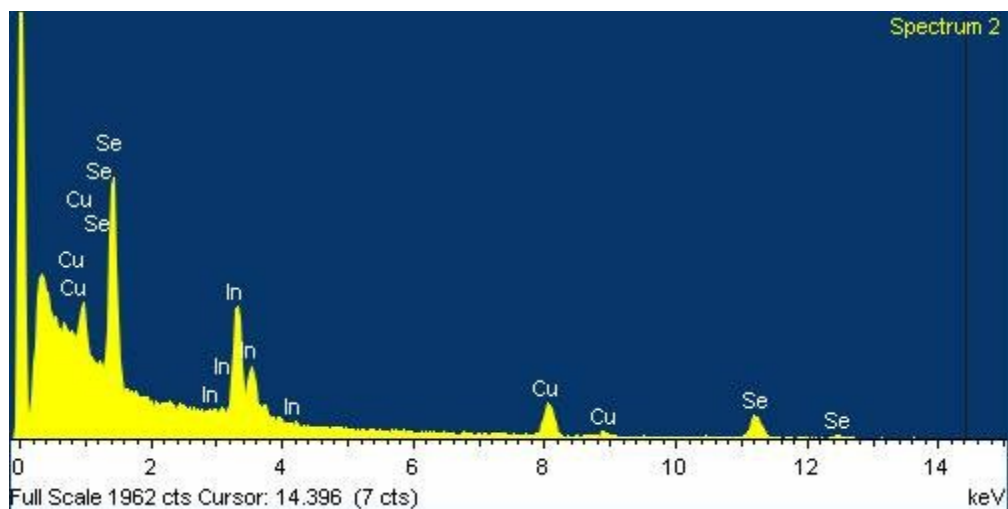


Figure S7: EDX spectrum of CuInSe_2 obtained from $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $300\text{ }^\circ\text{C}$ in OA for 30 min.

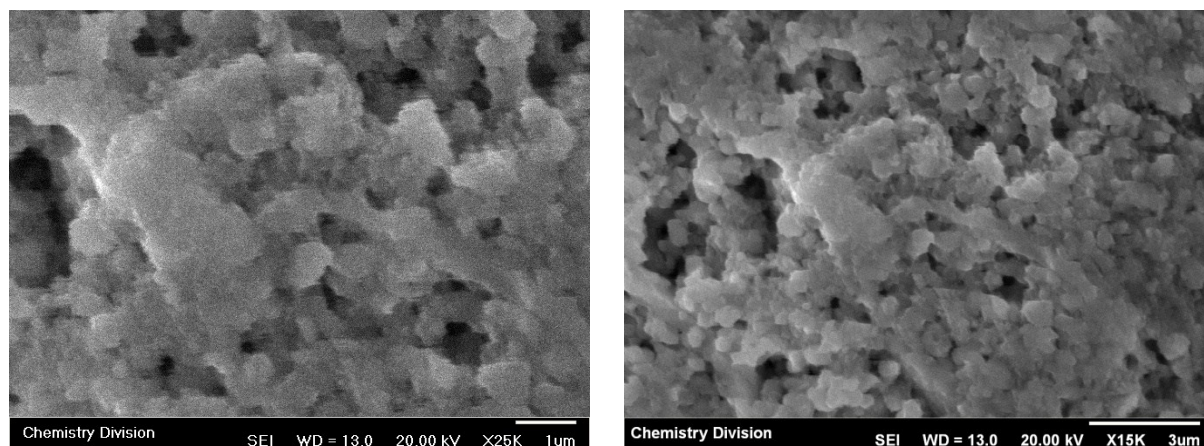


Figure S8: SEM images with different magnifications of CuInSe_2 obtained from $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $300\text{ }^\circ\text{C}$ in OA for 30 min.

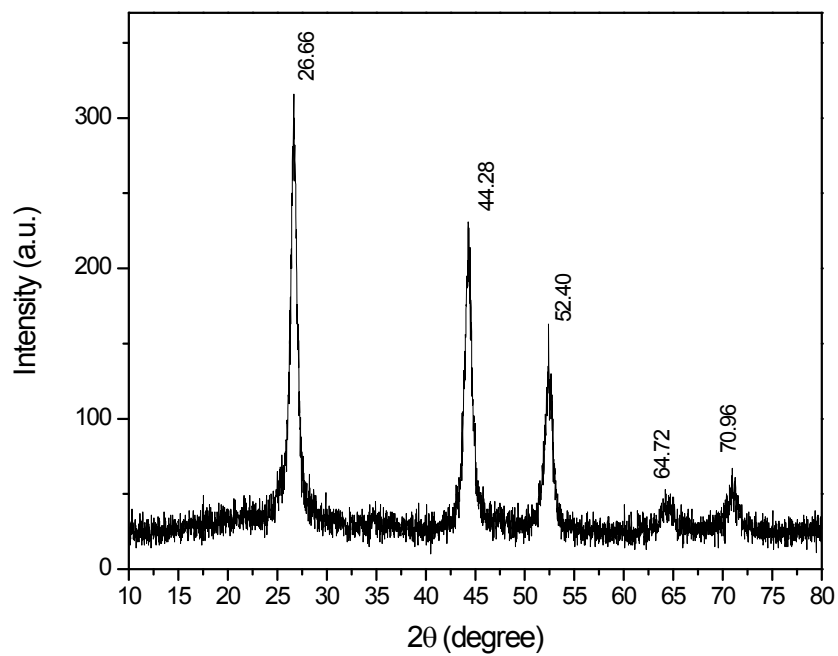


Figure S9: The PXRD pattern of CuInSe_2 obtained from thermolysis of $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ in hexadecylamine at 300 °C for 30 min.

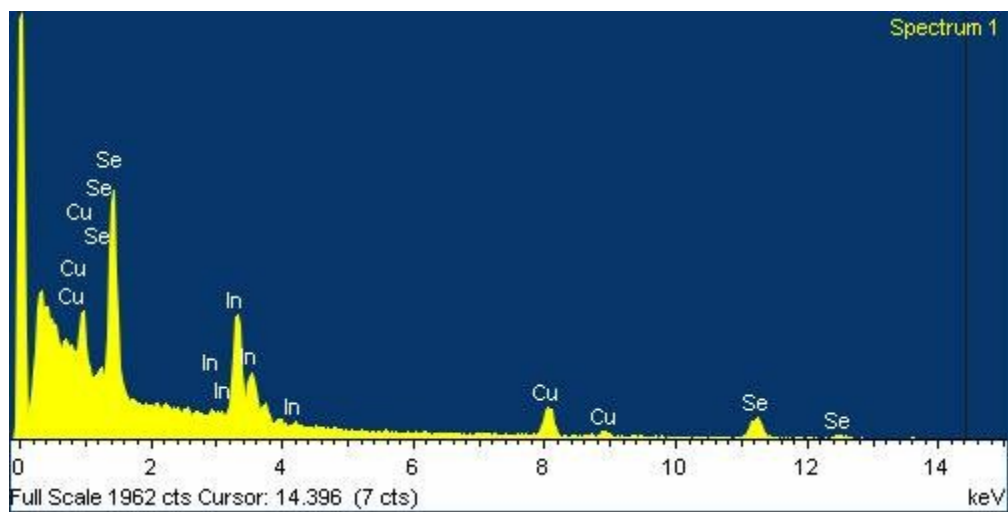


Figure S10: EDX spectrum of CuInSe_2 obtained from $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $300\text{ }^\circ\text{C}$ in HDA for 30 min.

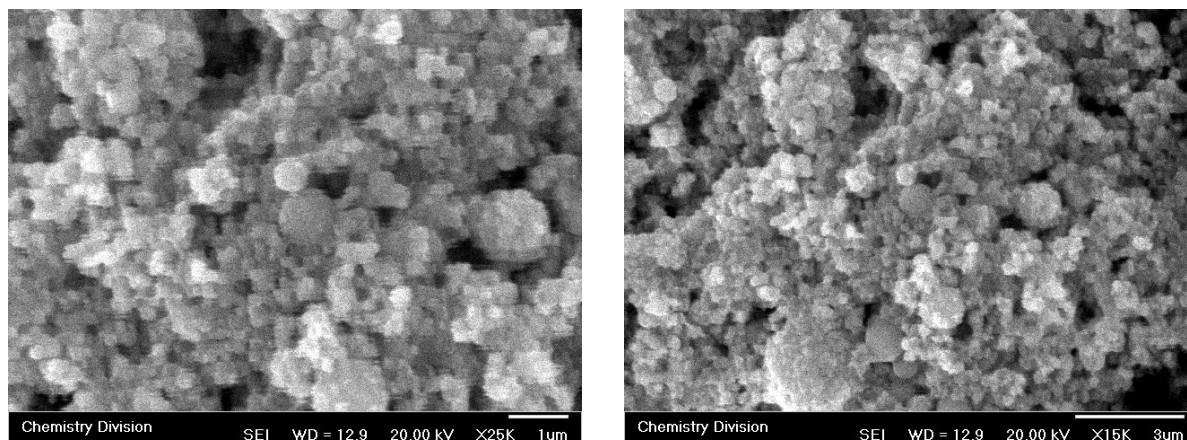


Figure S11: SEM images with different magnifications of CuInSe_2 obtained from $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $300\text{ }^\circ\text{C}$ in HDA for 30 min.

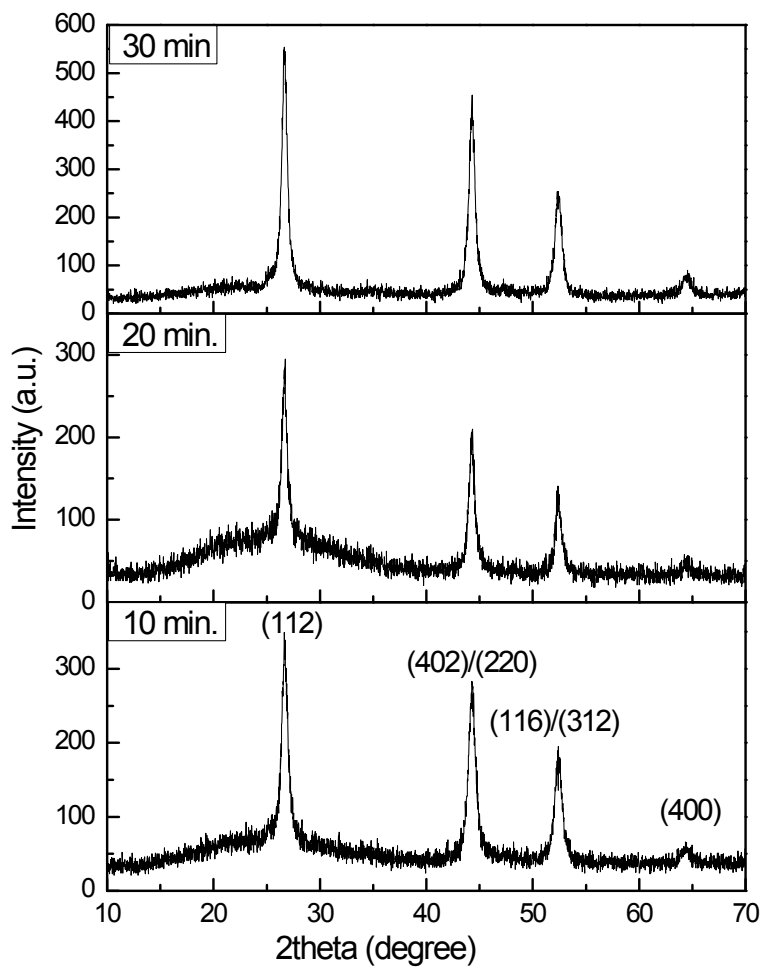


Figure S12: The PXRD pattern of CuInSe₂ obtained from thermolysis of [(PPh₃)₂CuIn(SeCH₂C₆H₅)₄] in OA at 300 °C for 10, 20 and 30 min.

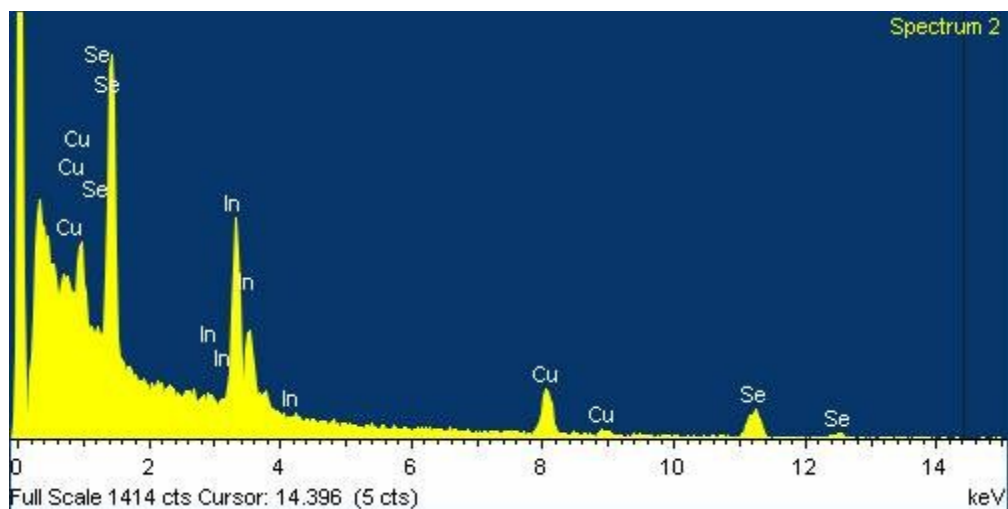


Figure S13: EDX spectrum of CuInSe_2 obtained from $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $300\text{ }^\circ\text{C}$ in OA for 10 min.

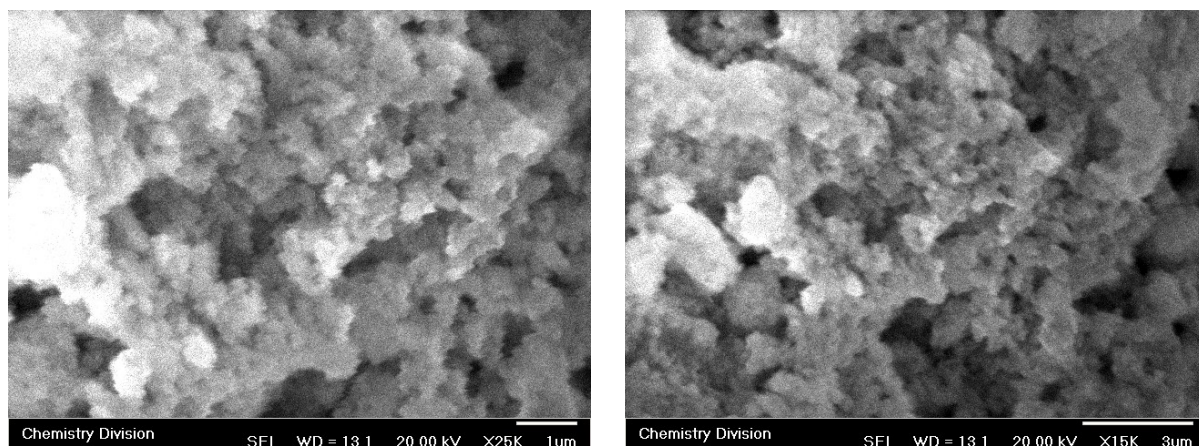


Figure S14: SEM images with different magnifications of CuInSe_2 obtained from $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ at $300\text{ }^\circ\text{C}$ in OA for 10 min.

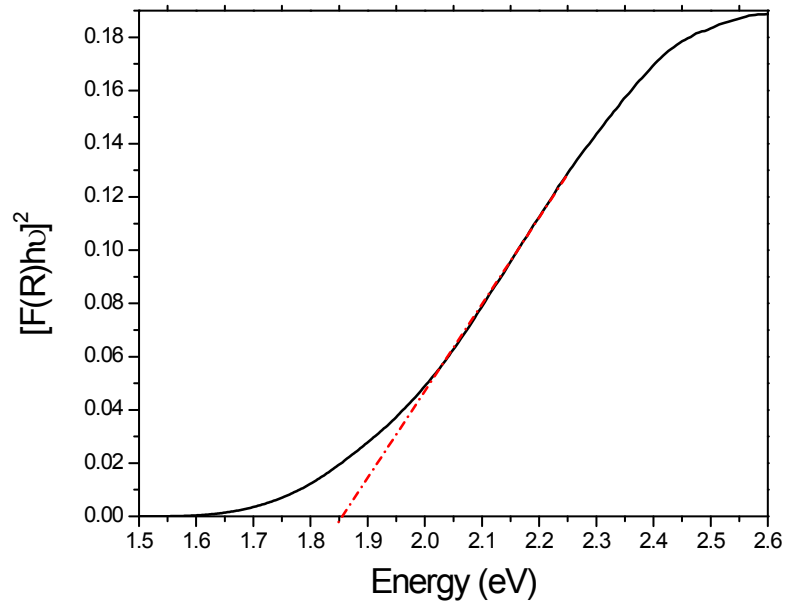


Figure S15: Plots of $[F(R)hv]^2$ vs energy generated by Kubelka-Munk transformation of solid-state diffuse reflectance data CuInSe_2 nanostructures obtained by thermolysis of $[(\text{PPh}_3)_2\text{CuIn}(\text{SeCH}_2\text{C}_6\text{H}_5)_4]$ in HDA at $300\text{ }^\circ\text{C}$ for a duration of 30 minutes.