Electronic Supplementary Information

A simple one pot synthesis of cubic Cu₃FeS₄

Prashant Kumarᵃ, Meenakshi Gusainᵃ, Pandian Senthil Kumarᵇ, Sitharaman Umaᵃ and Rajamani Nagarajan**

ᵃMaterials Chemistry Group, Department of Chemistry, University of Delhi, Delhi 110007, India

ᵇDepartment of Physics and Astrophysics, University of Delhi, Delhi 110007, India

*E-mail: rnagarajan@chemistry.du.ac.in
Fig. S1 PXRD pattern of product obtained from refluxing (a) 0.50 g (5 mmol) of CuCl with 0.76 g (10 mmol) thiourea, (b) FeCl₃ with thiourea and (c) CuCl, FeCl₃ and thiourea. JCPDS Files of Cu₁.₈S, Fe₃S₄ and cubic Cu₅FeS₄ are provided for easy comparison.

Fig. S2 EDX spectrum along with the analysis of synthesized cubic Cu₅FeS₄.
**Fig. S3** Room temperature Raman spectrum of Cu$_9$S$_5$ (Cu$_{1.8}$S) obtained by refluxing CuCl and thiourea in ethylene glycol.

**Fig. S4** PXRD pattern of the product from the reaction of (a) 0.50 g (5 mmol) CuCl, 1.01 g (0.25 mmol) of Fe$_2$(SO$_4$)$_3$ and 0.76 g (10 mmol) thiourea (b) 0.50 g (5 mmol) CuCl, 2.02 g (0.5 mmol) of Fe(NO$_3$)$_3$·9H$_2$O and 0.76 g (10 mmol) thiourea in 100 mL of ethylene glycol for 1.5 h. JCPDS files of Fe$_3$S$_4$, hexagonal CuS, Cu$_9$S$_5$ (Cu$_{1.8}$S) and cubic Cu$_5$FeS$_4$. 

S3
**Fig. S5** Comparison of the PXRD pattern of Cu$_5$FeS$_4$ with the known iron sulphide compositions in higher symmetry.