

Electronic Supplementary Information

A simple one pot synthesis of cubic Cu_5FeS_4

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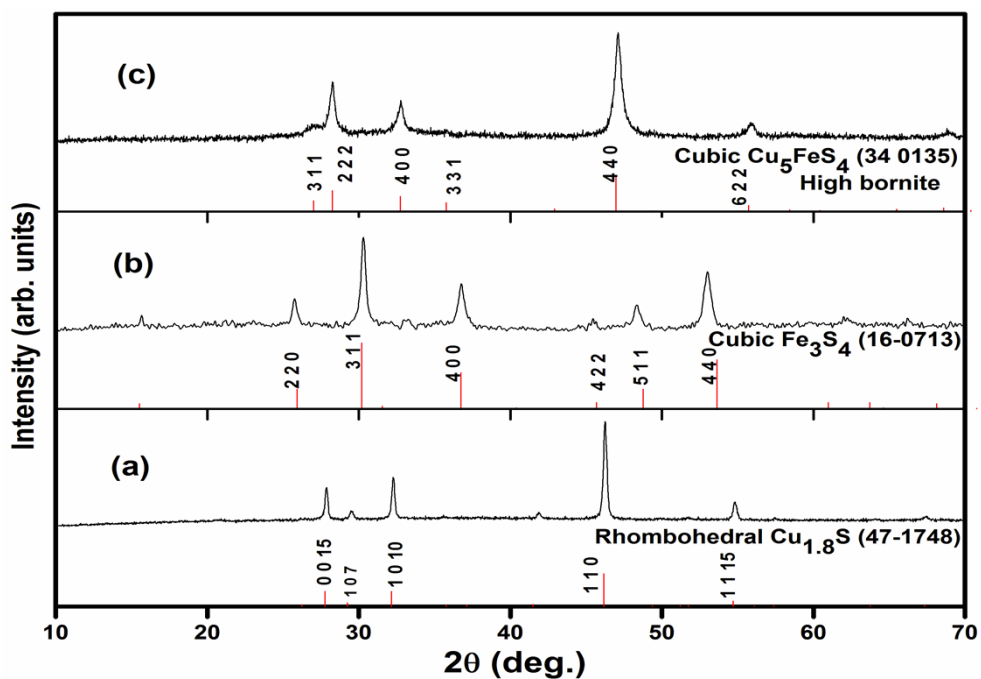


Fig. S1 PXRD pattern of product obtained from refluxing (a) 0.50 g (5 mmol) of CuCl with 0.76 g (10 mmol) thiourea, (b) FeCl₃ with thiourea and (c) CuCl, FeCl₃ and thiourea. JCPDS Files of Cu_{1.8}S, Fe₃S₄ and cubic Cu₅FeS₄ are provided for easy comparison.

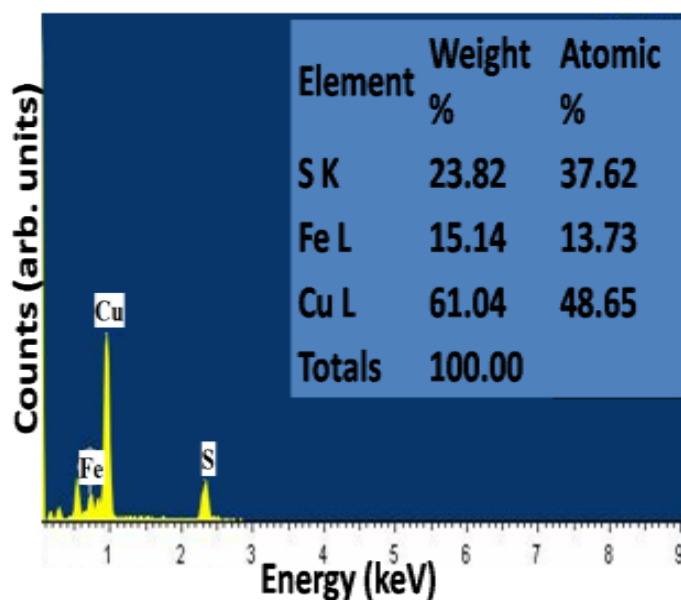


Fig. S2 EDX spectrum along with the analysis of synthesized cubic Cu₅FeS₄.

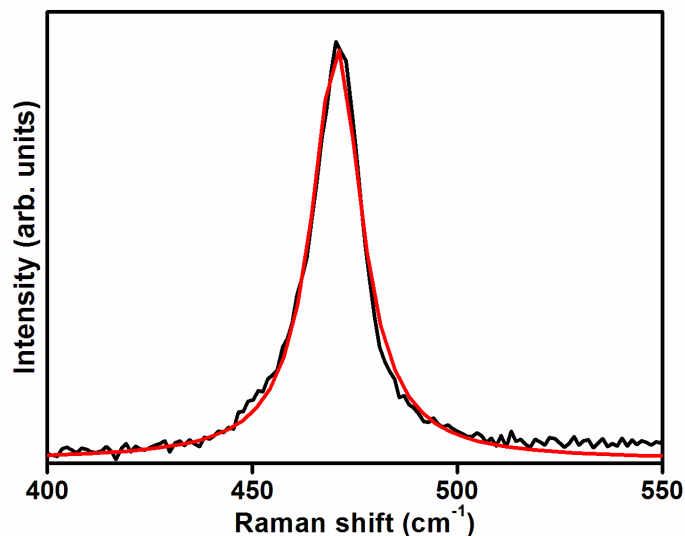


Fig.S3 Room temperature Raman spectrum of Cu_9S_5 ($\text{Cu}_{1.8}\text{S}$) obtained by refluxing CuCl and thiourea in ethylene glycol.

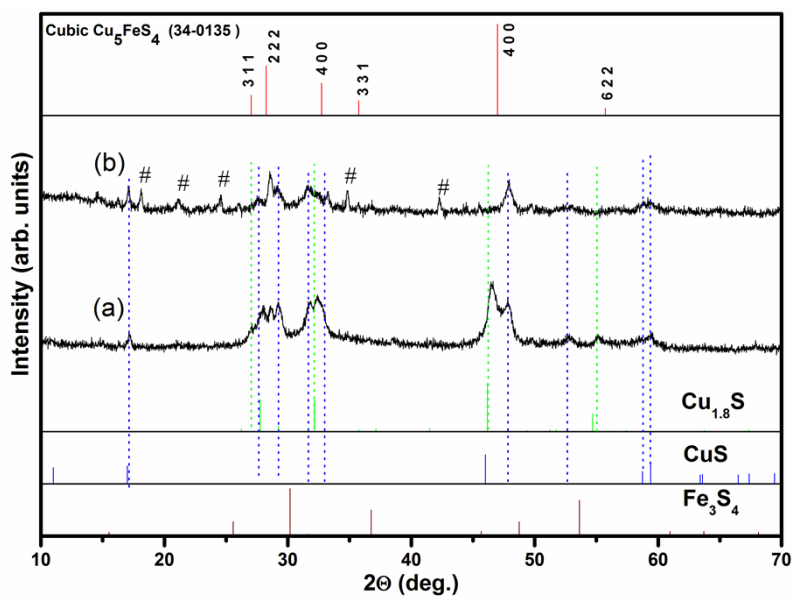


Fig. S4 PXRD pattern of the product from the reaction of (a) 0.50 g (5 mmol) CuCl , 1.01 g (0.25 mmol) of $\text{Fe}_2(\text{SO}_4)_3$ and 0.76 g (10 mmol) thiourea (b) 0.50 g (5 mmol) CuCl , 2.02 g (0.5 mmol) of $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and 0.76 g (10 mmol) thiourea in 100 mL of ethylene glycol for 1.5 h. JCPDS files of Fe_3S_4 , hexagonal CuS , Cu_9S_5 ($\text{Cu}_{1.8}\text{S}$) and cubic Cu_5FeS_4 .

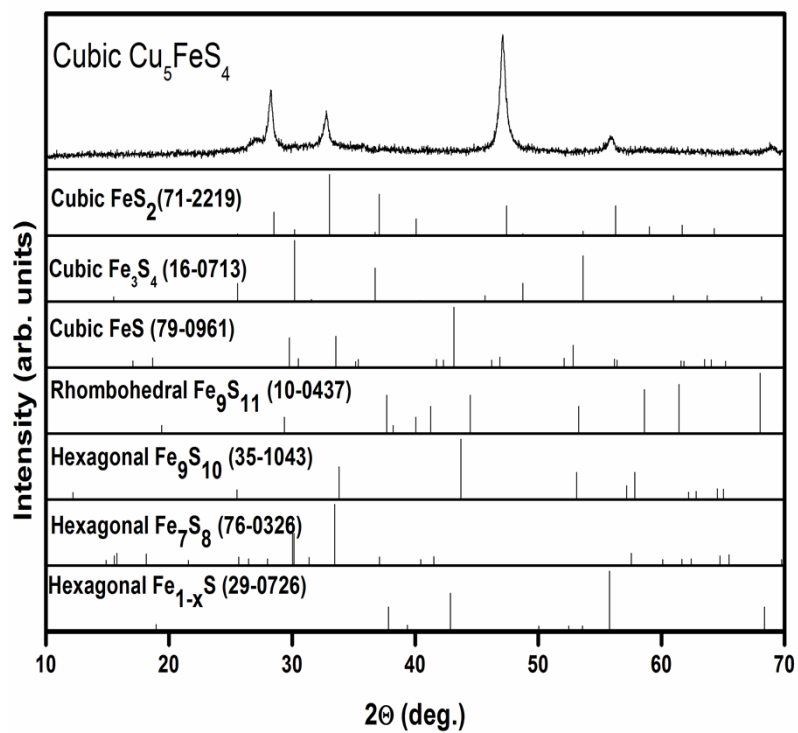


Fig. S5 Comparison of the PXRD pattern of Cu_5FeS_4 with the known iron sulphide compositions in higher symmetry.