Effect of Anion Substitution on the Structural and Transport Properties of Argyrodites $Cu_7PSe_{6-x}S_x$

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Supporting Information

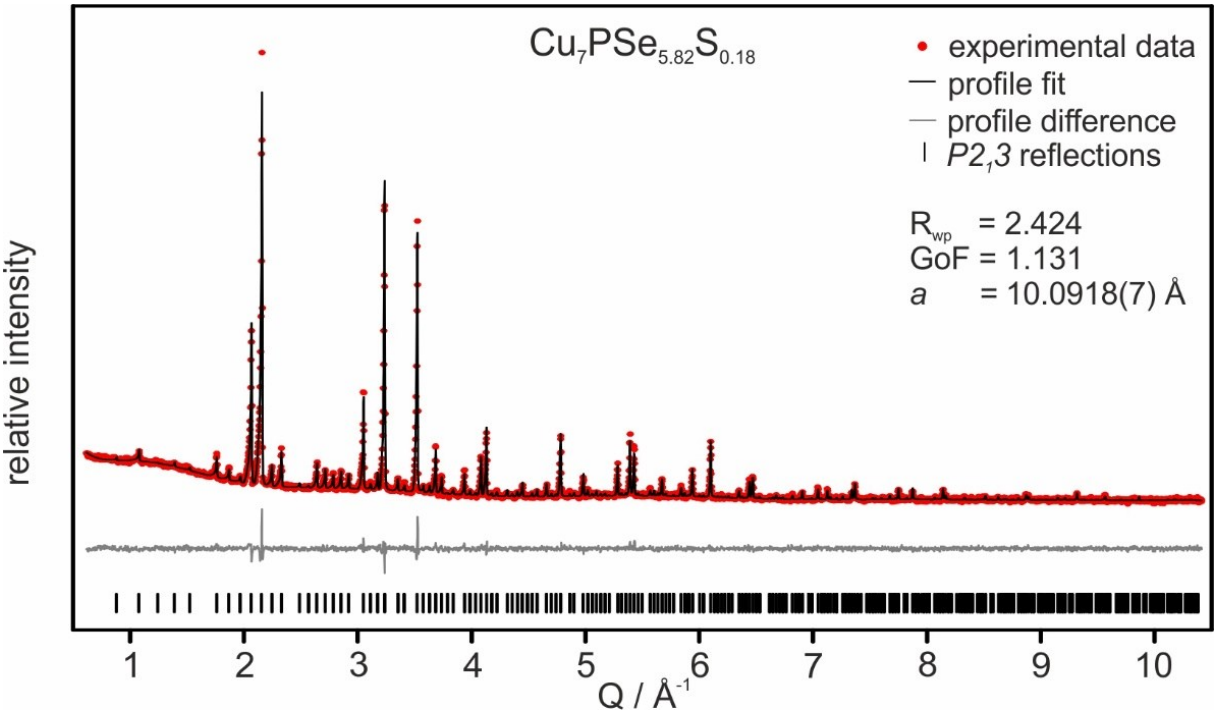

Figure S1. Rietveld refinement of $Cu_7PSe_{5.82}S_{0.18}$.

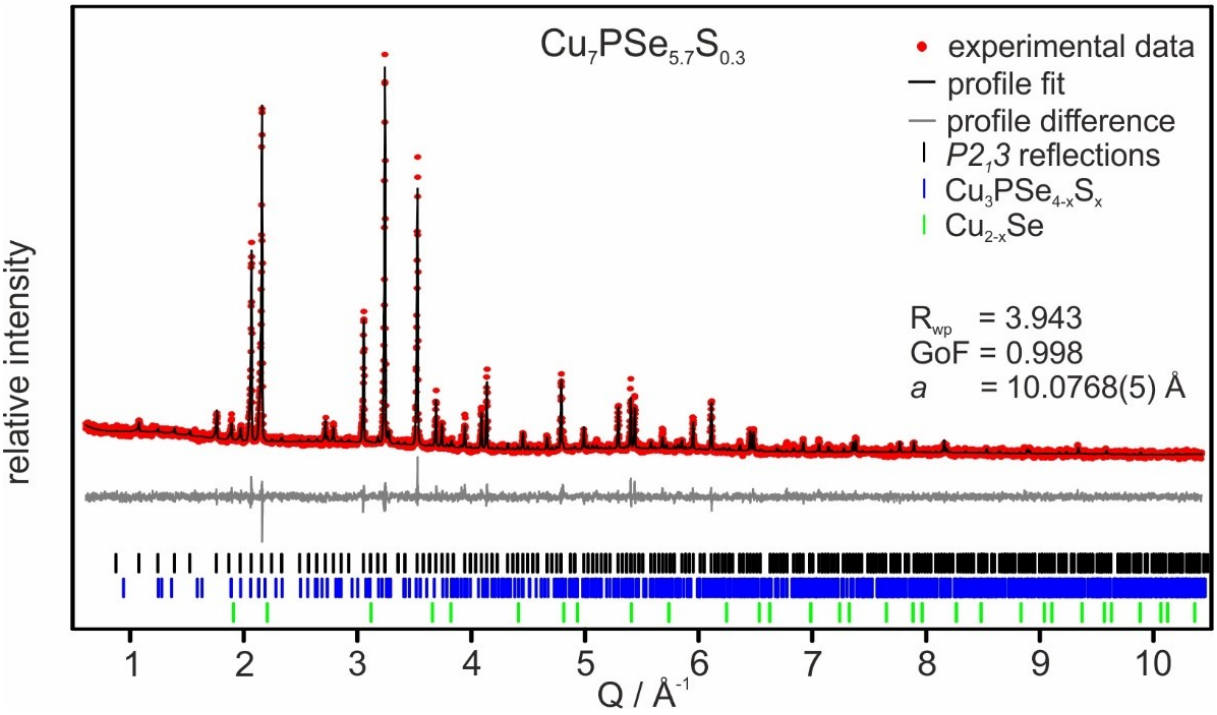

Figure S2. Rietveld refinement of $Cu_7PSe_{5.7}S_{0.3}$.

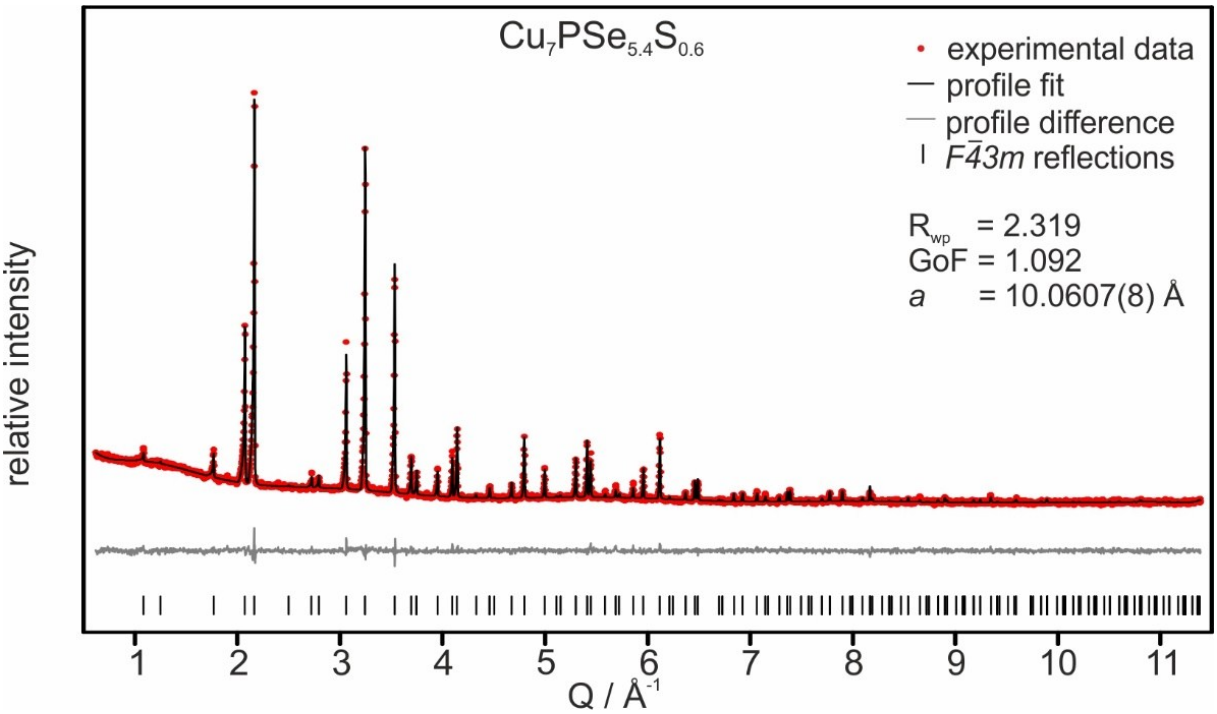

Figure S3. Rietveld refinement of $Cu_7PSe_{5.4}S_{0.6}$.

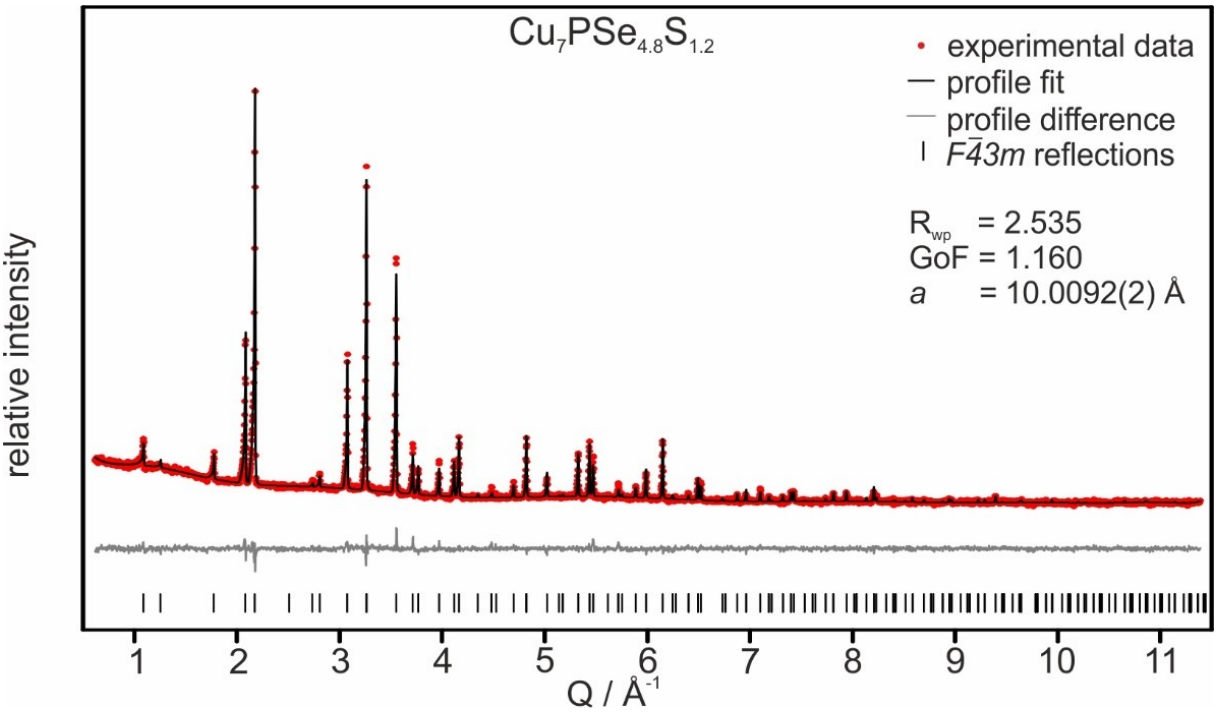

Figure S4. Rietveld refinement of $Cu_7PSe_{4.8}S_{1.2}$.

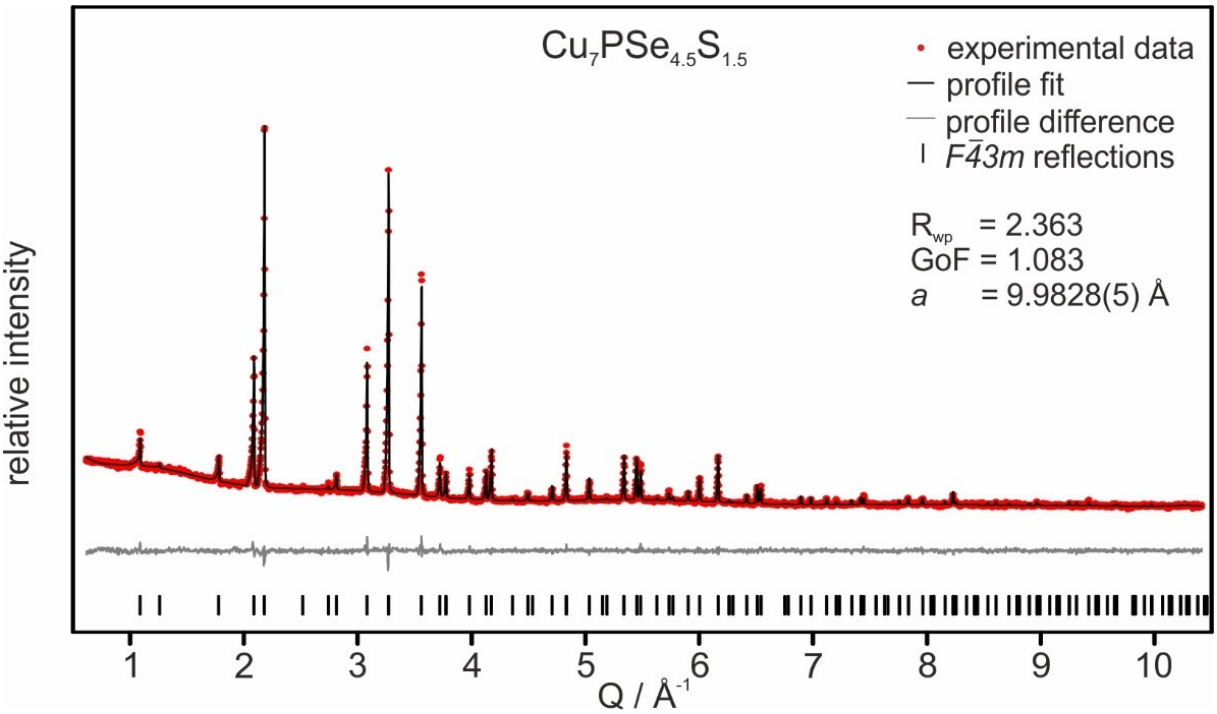

Figure S5. Rietveld refinement of $Cu_7PSe_{4.5}S_{1.5}$.

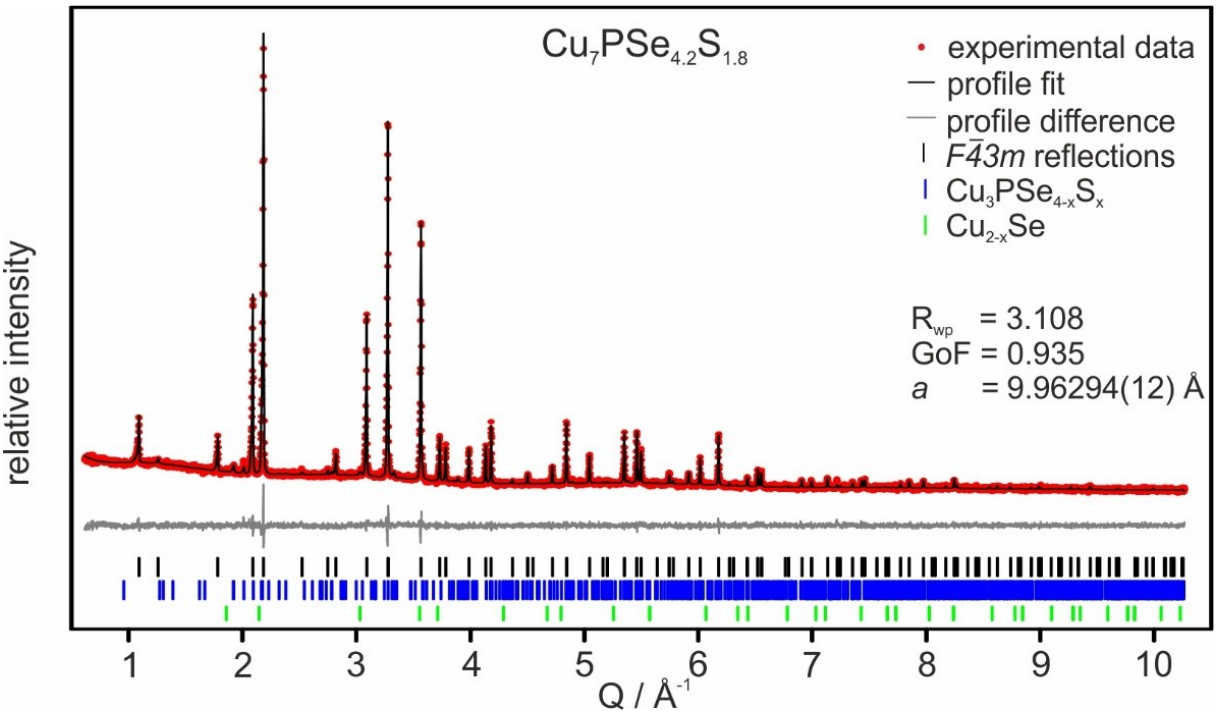

Figure S6. Rietveld refinement of $Cu_7PSe_{4.2}S_{1.8}$.

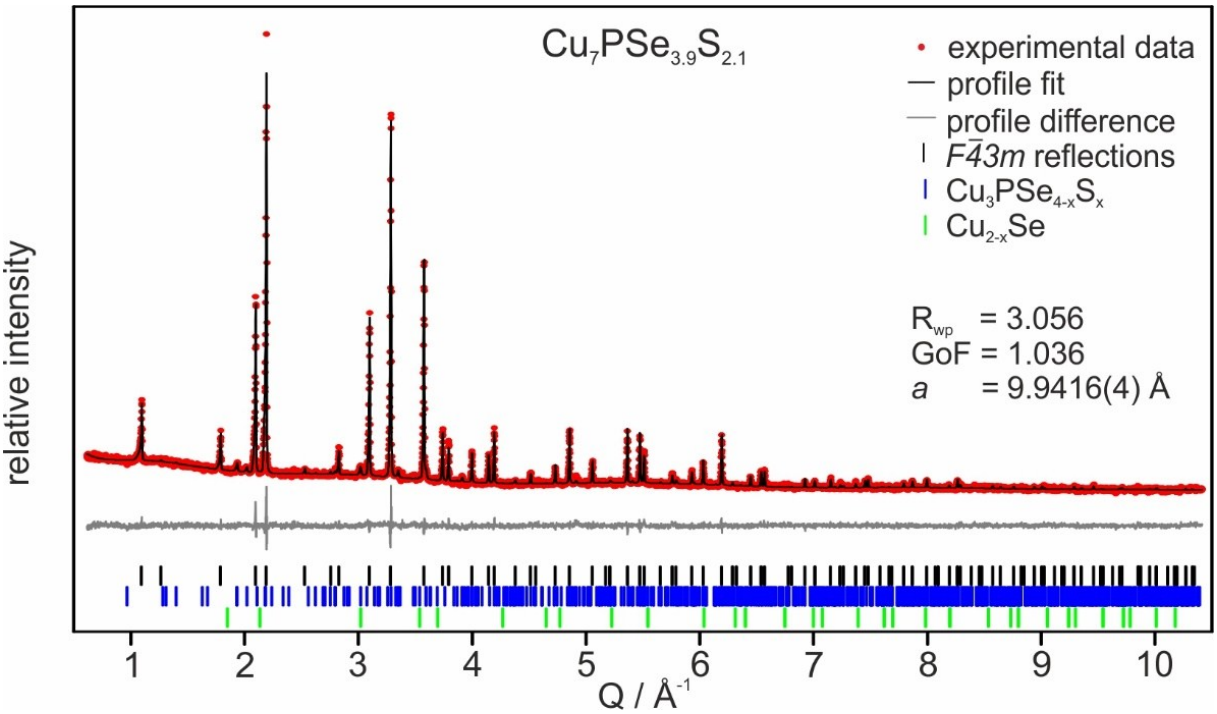

Figure S7. Rietveld refinement of $Cu_7PSe_{3.9}S_{2.1}$.

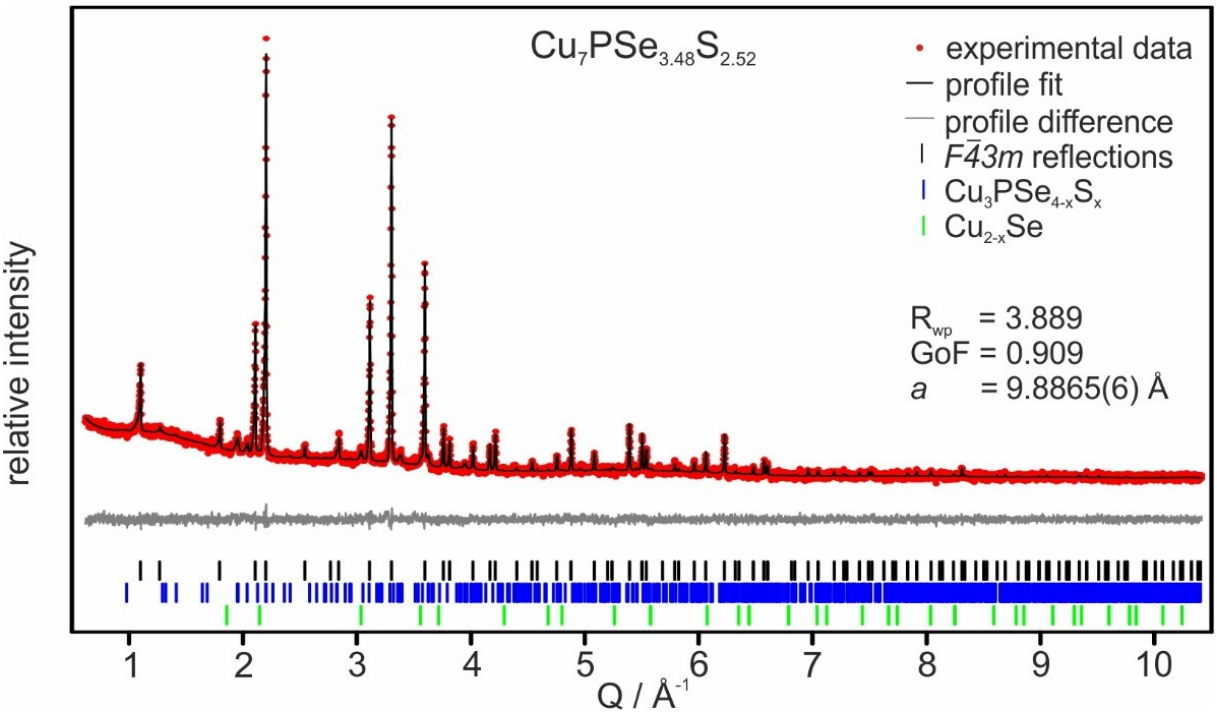

Figure S8. Rietveld refinement of $Cu_7PSe_{3.48}S_{2.52}$.

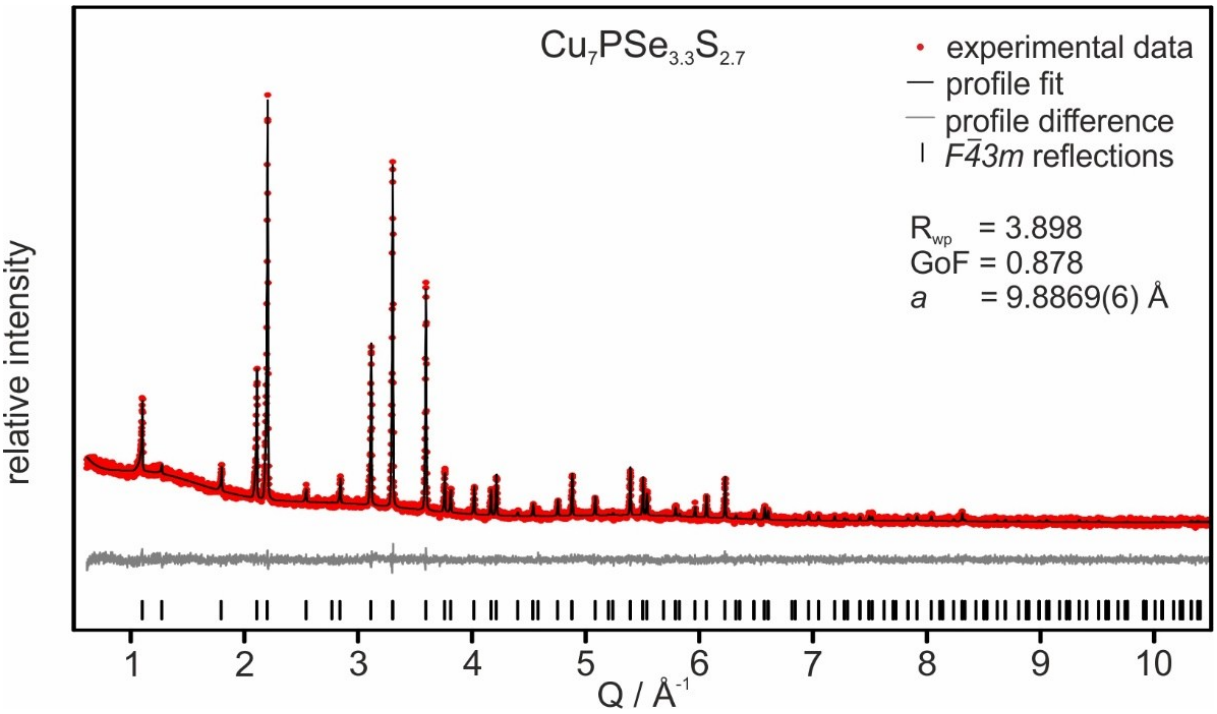

Figure S9. Rietveld refinement of $Cu_7PSe_{3.3}S_{2.7}$.

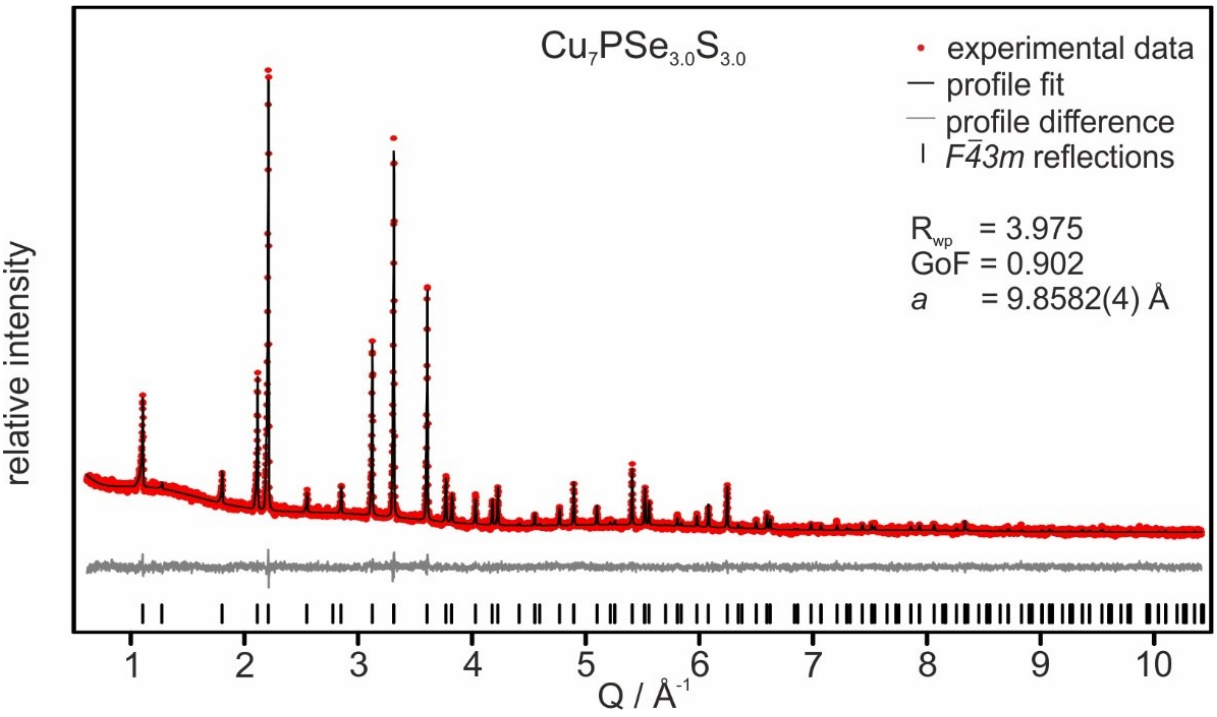

Figure S10. Rietveld refinement of $Cu_7PSe_{3.0}S_{3.0}$.

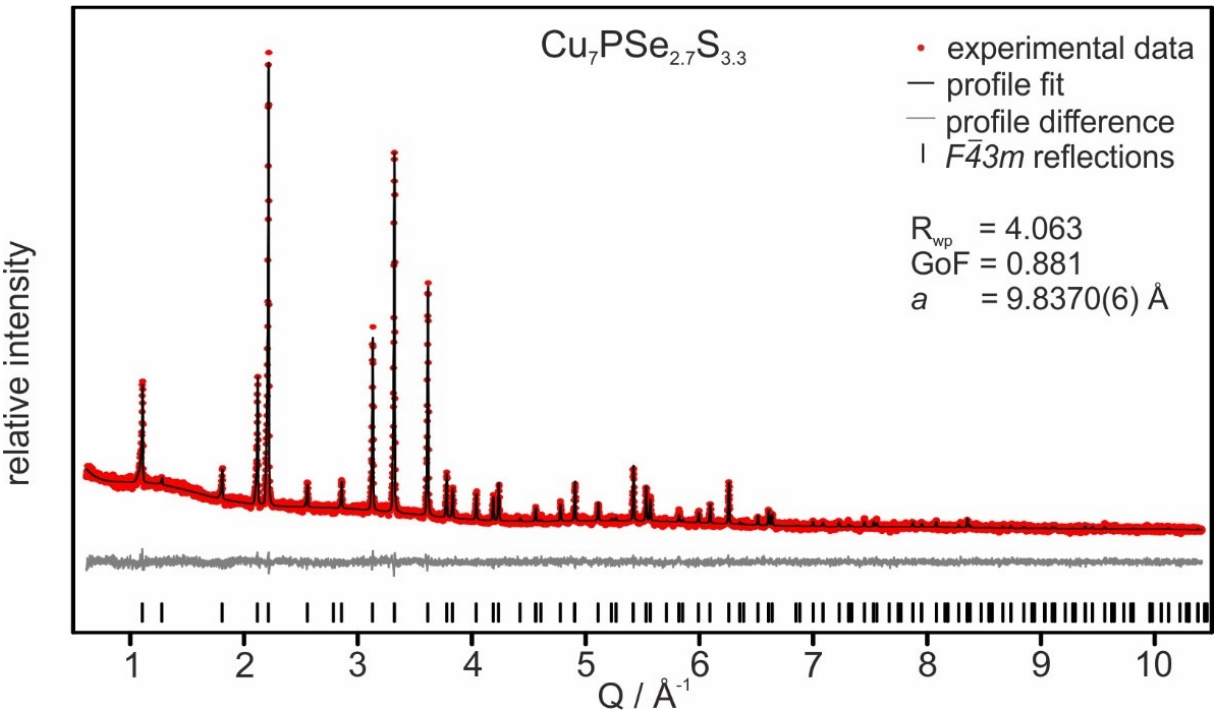

Figure S11. Rietveld refinement of $Cu_7PSe_{2.7}S_{3.3}$.

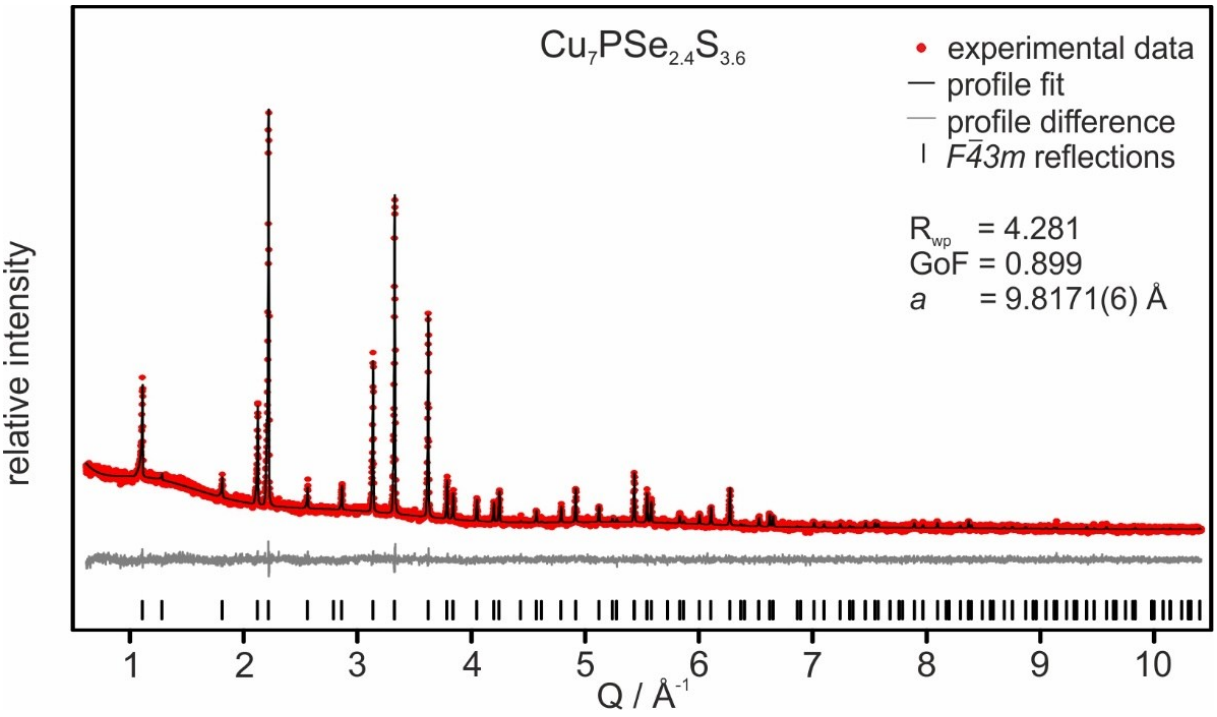

Figure S12. Rietveld refinement of $Cu_7PSe_{2.4}S_{3.6}$.

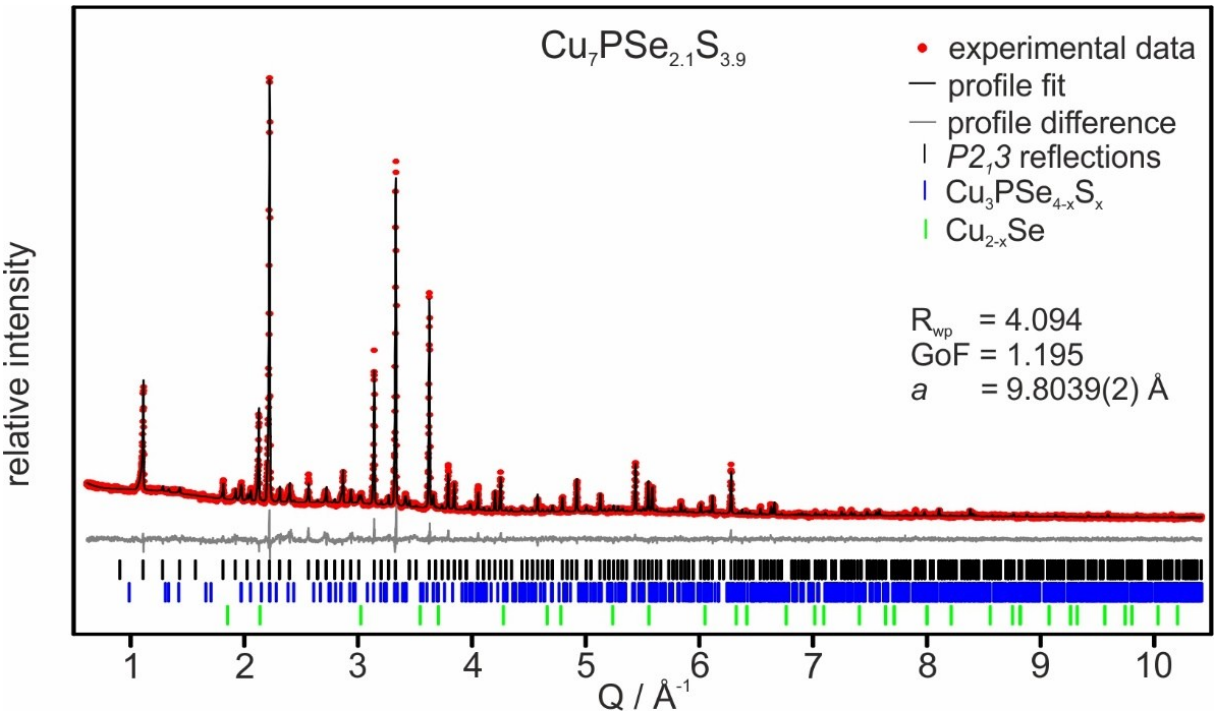

Figure S13. Rietveld refinement of $Cu_7PSe_{2.1}S_{3.9}$.

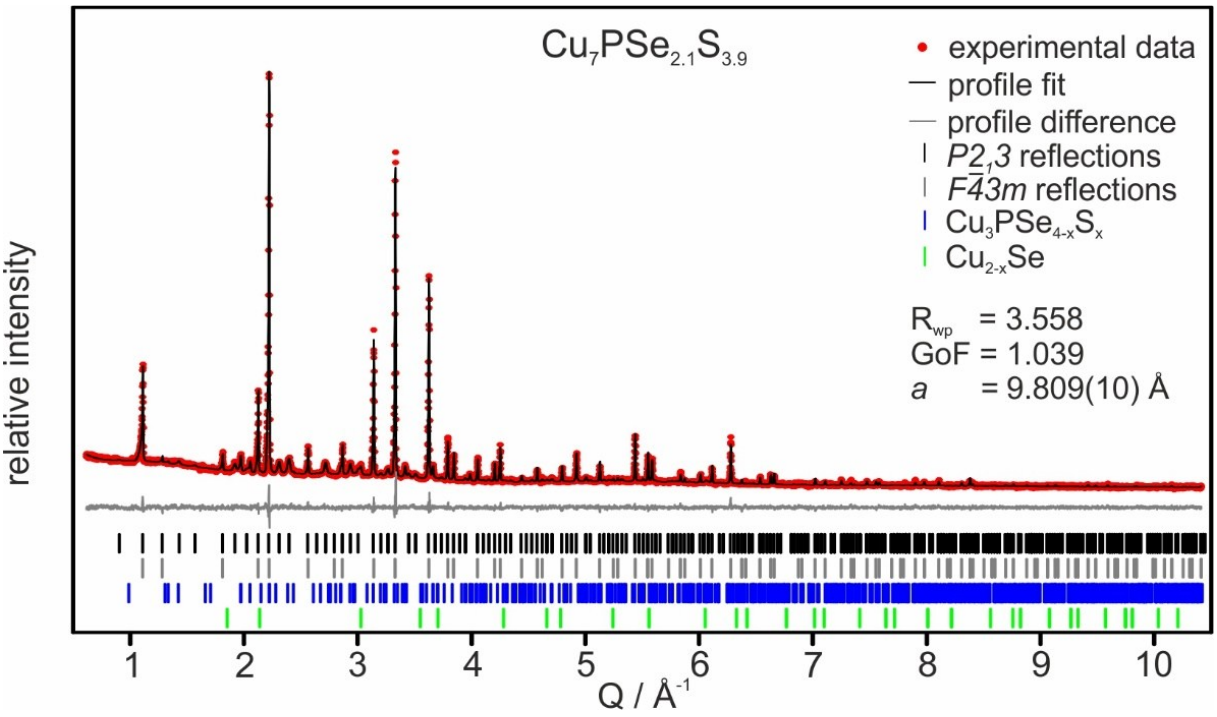

Figure S14. Rietveld refinement of $Cu_7PSe_{2.1}S_{3.9}$.

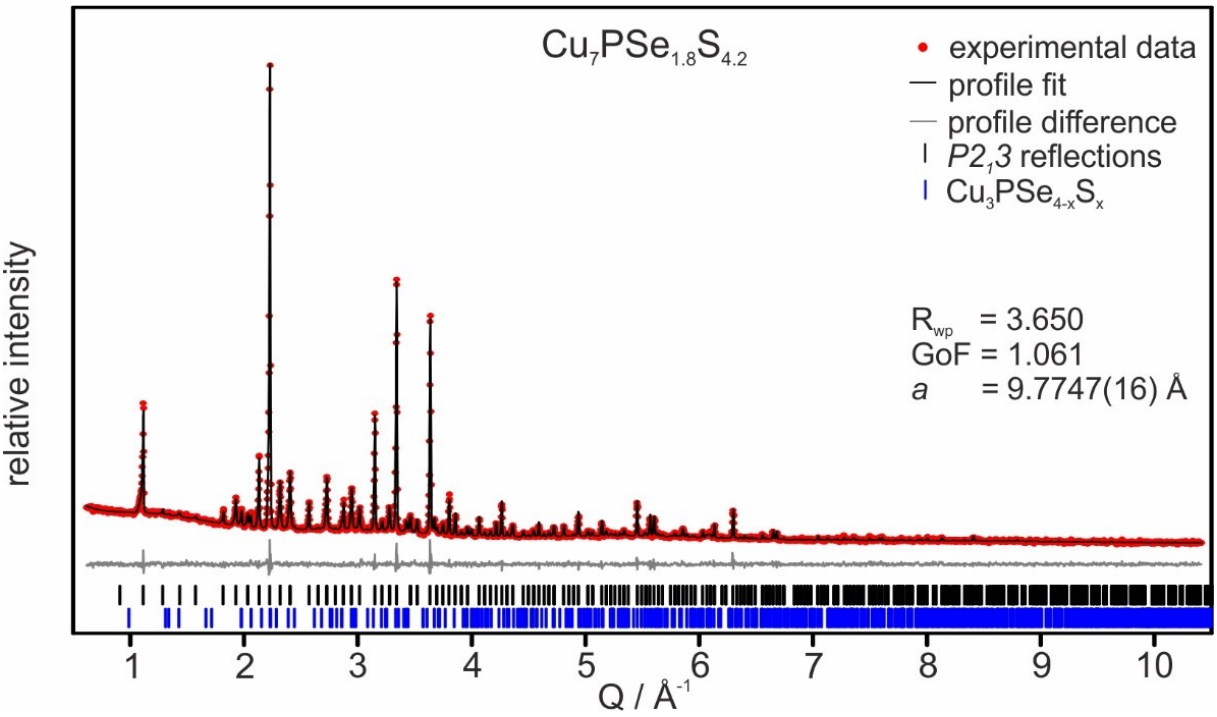

Figure S15. Rietveld refinement of $Cu_7PSe_{1.8}S_{4.2}$.

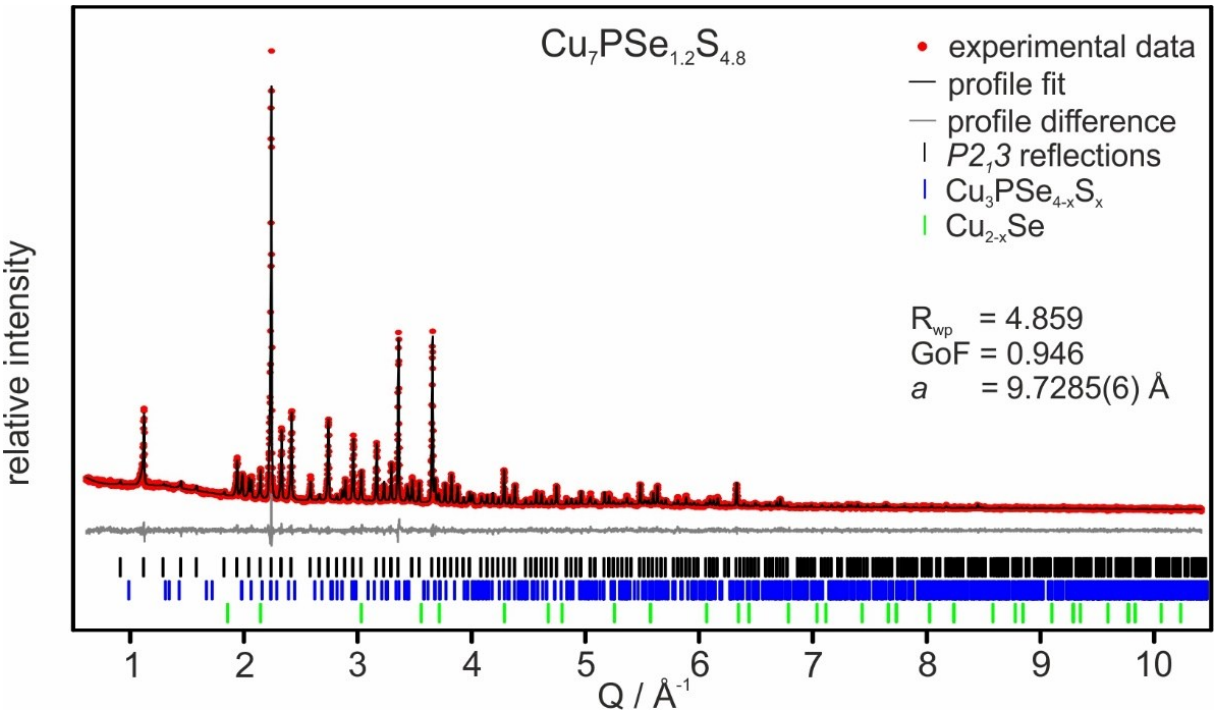

Figure S16. Rietveld refinement of $Cu_7PSe_{1.2}S_{4.8}$.

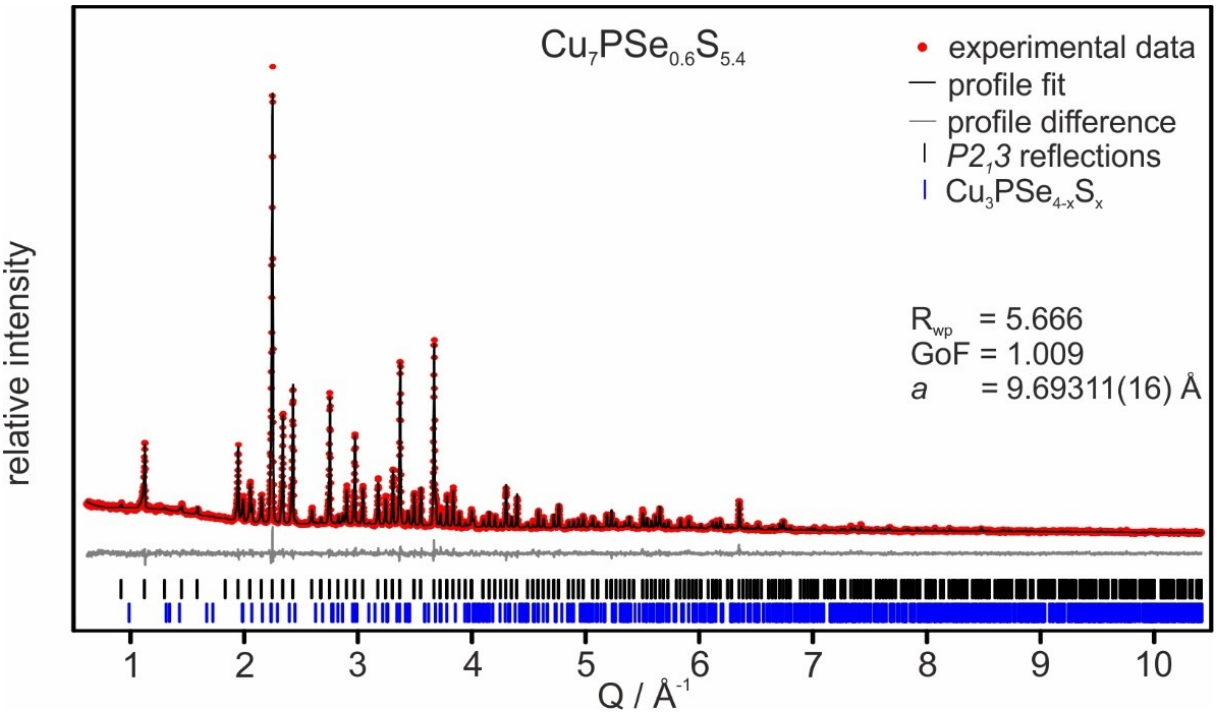

Figure S17. Rietveld refinement of $Cu_7PSe_{0.6}S_{5.4}$.

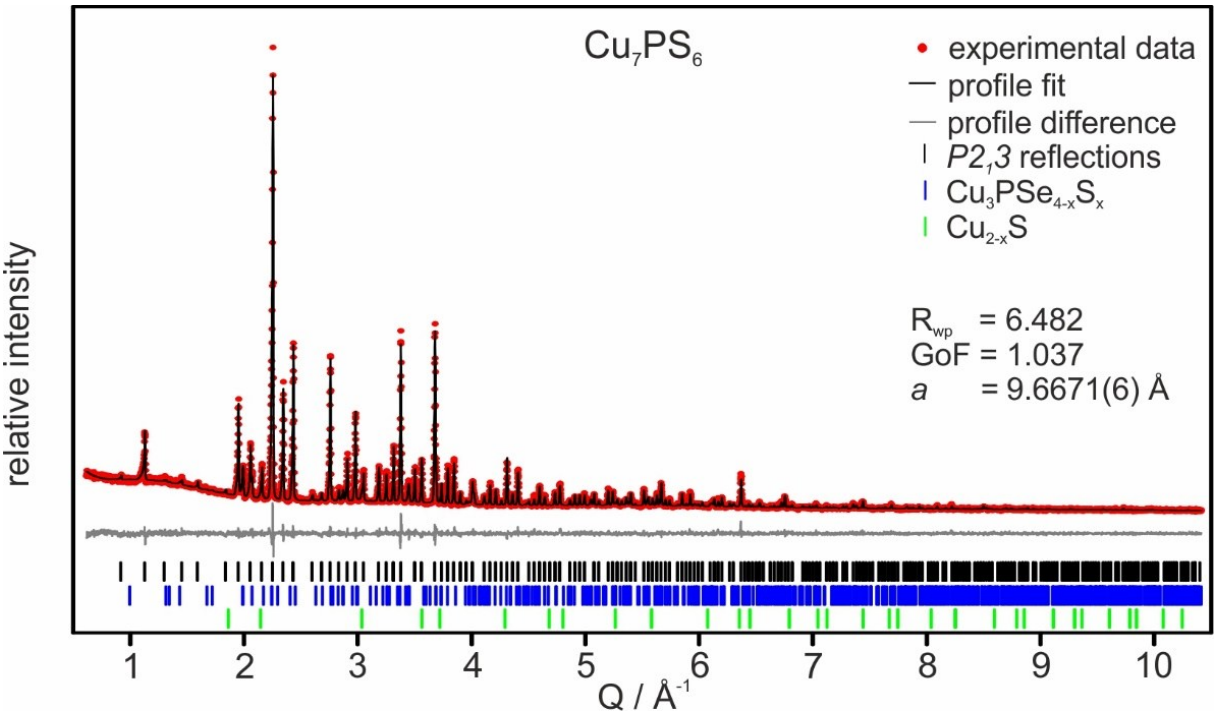

Figure S18. Rietveld refinement of Cu_7PS_6.

Table S1. Refined compositions of the synthesized samples and minor contaminants.

$x_{nom.}$	x_{real}	S %	SG	$Cu_7PSe_{6-x}S_x$	$Cu_3PSe_{4-x}S_x$	$Cu_2Se_{1-x}S_x$
0.18	0.20	3 %	$P2_13$	100%	-	-
0.30	0.30	5%	$P2_13$	92.13%	7.36%	0.51%
0.60	0.50	10%	$F\bar{4}3m$	100%	-	-
1.20	1.20	20%	$F\bar{4}3m$	100%	-	-
1.50	1.50	25%	$F\bar{4}3m$	100%	-	-
1.80	1.83	30%	$F\bar{4}3m$	95.19%	4.42%	0.39%
2.10	2.13	35%	$F\bar{4}3m$	96.16%	2.93%	0.91%
2.52	2.57	42%	$F\bar{4}3m$	90.64%	6.46%	2.90%
2.70	2.71	45%	$F\bar{4}3m$	100%	-	-
3.00	3.00	50%	$F\bar{4}3m$	100%	-	-
3.30	3.34	55%	$F\bar{4}3m$	100%	-	-
3.60	3.62	60%	$F\bar{4}3m$	100%	-	-
3.90	3.86	65%	$P2_13$	94.94%	4.08%	0.98%
4.20	4.19	70%	$P2_13$	97.20%	2.80%	-
4.80	4.79	80%	$P2_13$	93.06%	6.57%	0.37%
5.40	5.26	90%	$P2_13$	91.57%	8.43%	-
6.00	5.99	100%	$P2_13$	86.26%	12.49%	1.25%