

Low temperature thermoelectric and magnetoresistive properties of $Tl_2Cu_3FeQ_4$ ($Q= S, Se, Te$)

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Supporting information

Crystallographic details (Rietveld method) of $Tl_2Cu_3FeQ_4$ ($Q= S, Se, Te$)

Table S1: Crystallographic information

	$Tl_2Cu_3FeS_4$	$Tl_2Cu_3FeSe_4$	$Tl_2Cu_3FeTe_4$
$a=b$ (Å)	3.8650 (1)	3.9688 (1)	4.1289 (1)
c (Å)	13.1684 (2)	13.6914 (3)	14.7629 (1)
Cell Volume (Å ³)	196.71 (1)	215.66 (1)	251.68 (1)
Symmetry	tetragonal	tetragonal	Tetragonal
Space group	<i>I 4/mmm</i>	<i>I 4/mmm</i>	<i>I 4/mmm</i>
wRp (%)	7.24	6.66	7.63
Rp (%)	5.28	4.93	5.84
χ^2	1.764	1.706	1.492

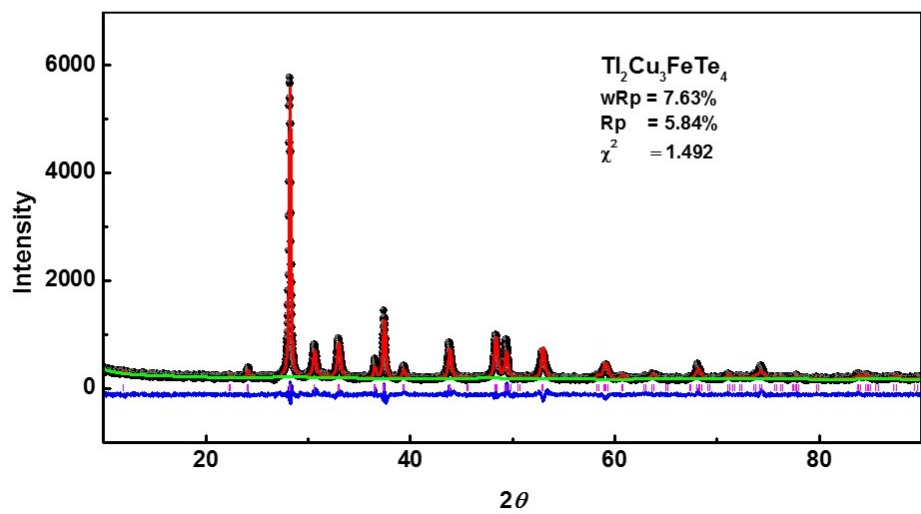
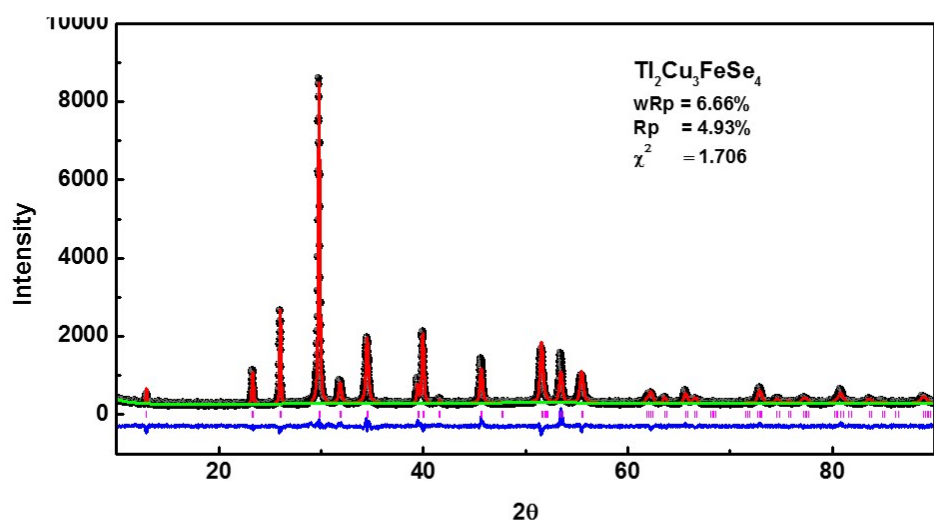
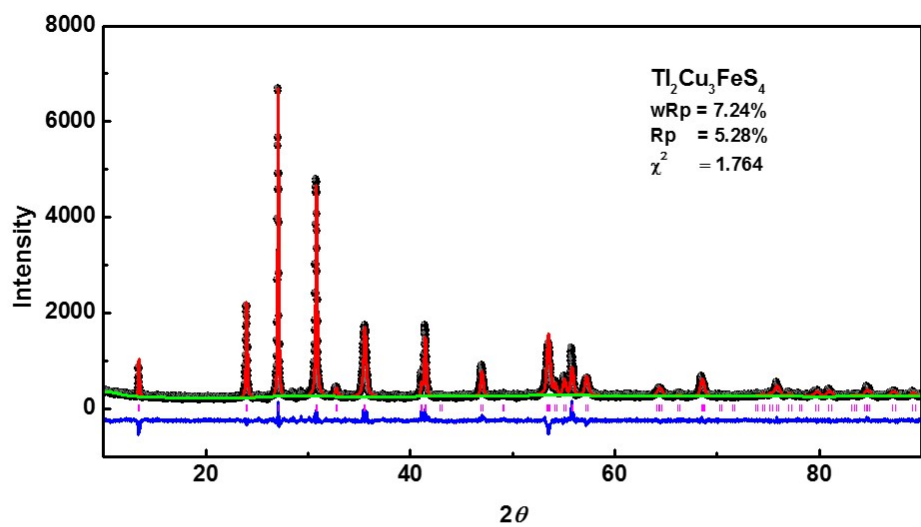


Figure S1: Rietveld fit of the powder XRD patterns for the three compositions as labelled. The XRD of the sulfide sample contains some minor peaks within the region $2\theta = 27$ to 29 degrees, corresponding to 100% peaks of $TlCuS_2$ and $CuFeS_2$ respectively.

Table S2: Atomic coordinates

Tl ₂ Cu ₃ FeS ₄				
Atom	Wyckoff	x, y, z	SOF	U _{iso}
Tl1	2a	0.0, 0.0, 0.0	1.0	0.0250
Cu1	4d	0.0, 0.5, 0.25	0.75	0.0055
Fe1	4d	0.0, 0.5, 0.25	0.25	0.0058
S1	4e	0.0, 0.0, 0.35133	1.0	0.0009
Tl ₂ Cu ₃ FeSe ₄				
Atom	Wyckoff	x, y, z	SOF	U _{iso}
Tl1	2a	0.0, 0.0, 0.0	1.0	0.0149
Cu1	4d	0.0, 0.5, 0.25	0.75	0.0135
Fe1	4d	0.0, 0.5, 0.25	0.25	0.0373
Se1	4e	0.0, 0.0, 0.35763	1.0	0.0132
Tl ₂ Cu ₃ FeTe ₄				
Atom	Wyckoff	x, y, z	SOF	U _{iso}
Tl1	2a	0.0, 0.0, 0.0	1.0	0.0011
Cu1	4d	0.0, 0.5, 0.25	0.75	0.0091
Fe1	4d	0.0, 0.5, 0.25	0.25	0.0091
Te1	4e	0.0, 0.0, 0.36194	1.0	0.0003

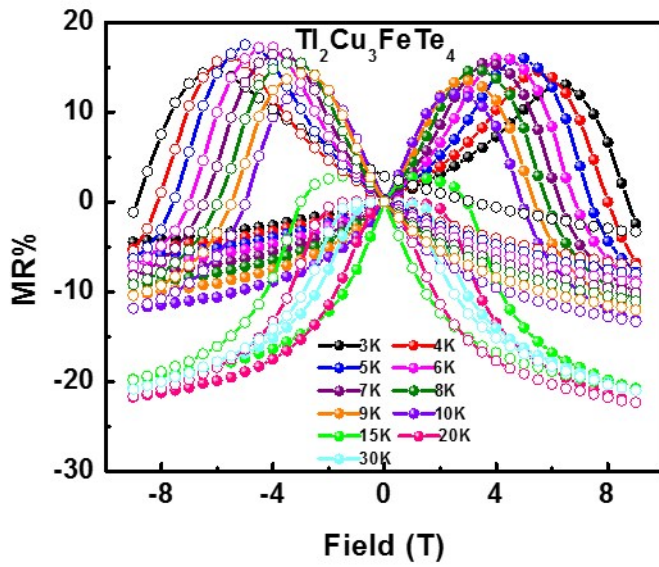


Figure S2: Magnetoresistance of the telluride measured at various temperatures. Closed symbols represent field sweep from -9 to +9 T and open symbols represent +9T to -9T, for every 0.5 T steps.