

Electronic Supporting Information

for the manuscript

Nickel - p-block Metal Mixed Chalcogenides Based on the AuCu₃-type Fragments: Iodine-assisted Synthesis as a Way of Obtaining New Structures

by

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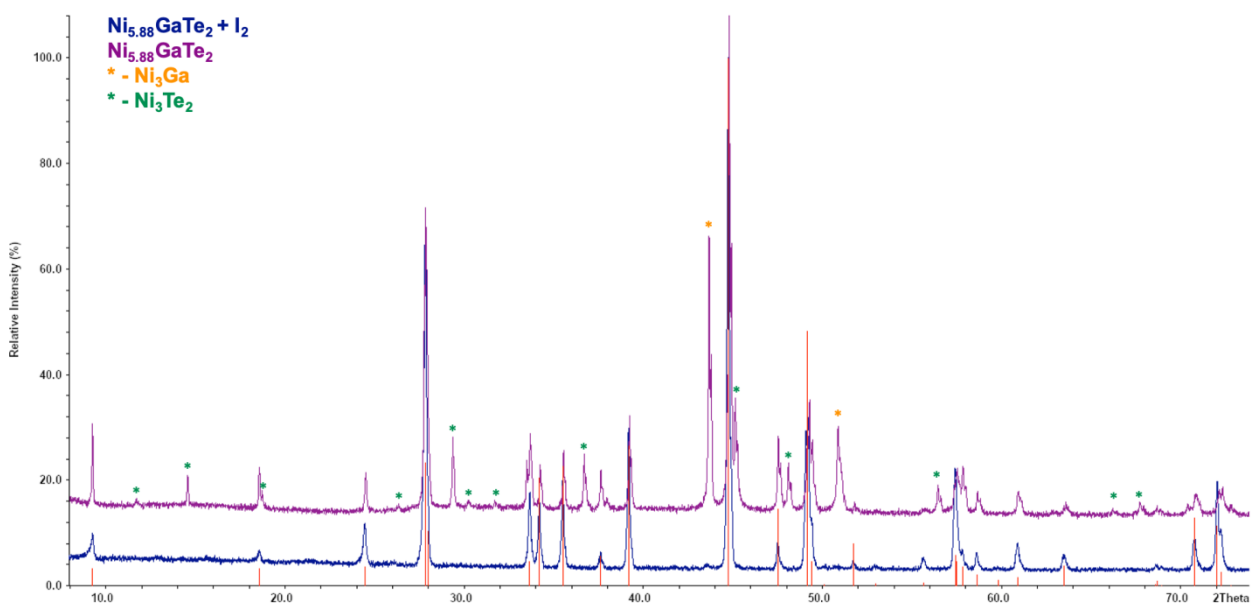


Figure S1. The effect of iodine on phase purity of Ni_{5.80}GaTe₂.

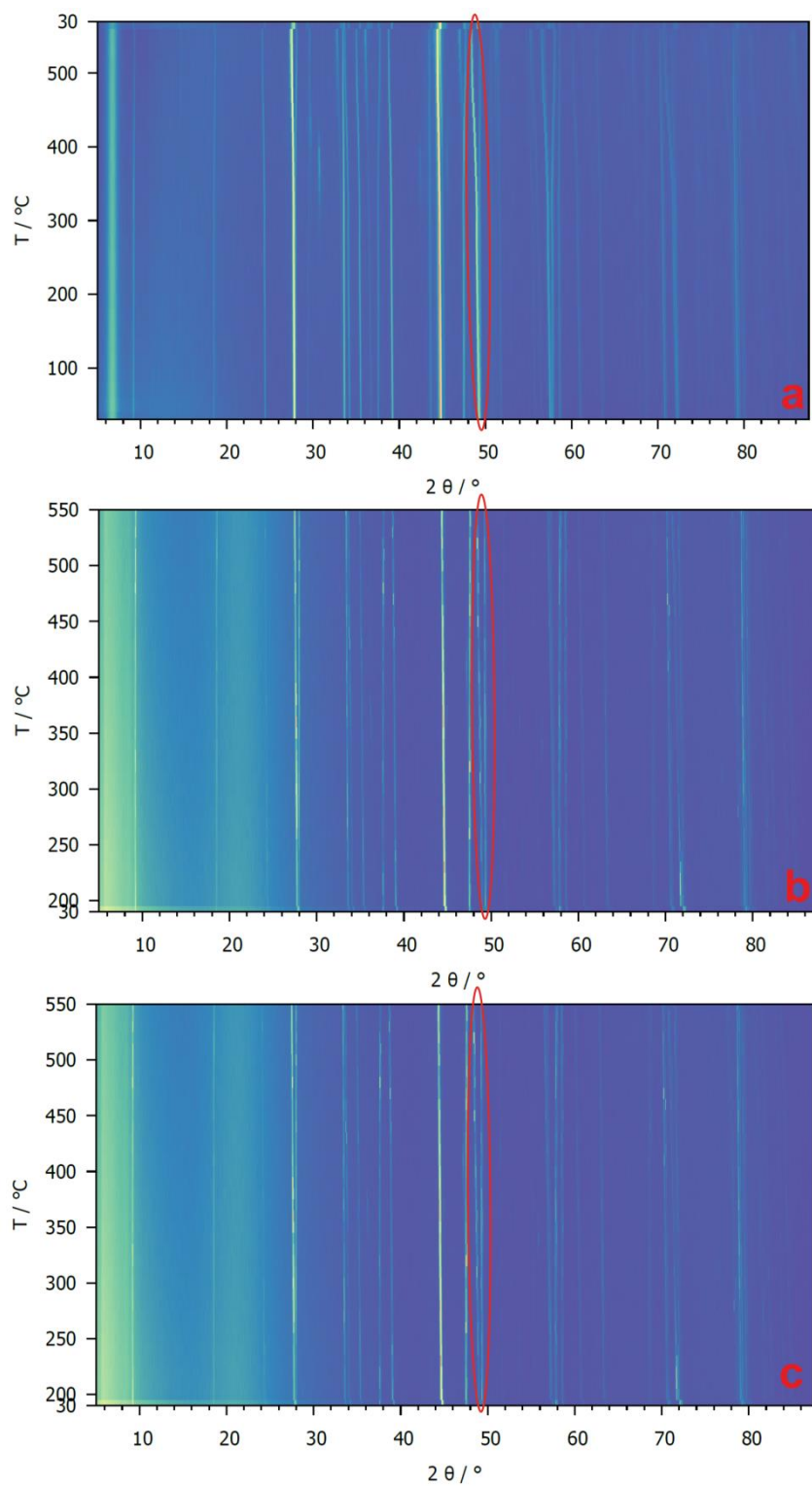


Figure S2. 2D in situ XRD patterns for $\text{Ni}_{5.80}\text{GaTe}_2$: a – flat sample under N_2 atmosphere, b – pressurized (750 Torr) capillary under N_2 atmosphere, c - pressurized capillary under ca. 53 kTorr H_2 atmosphere. Red ellipse encircles the 200 – 020 pair of reflections.

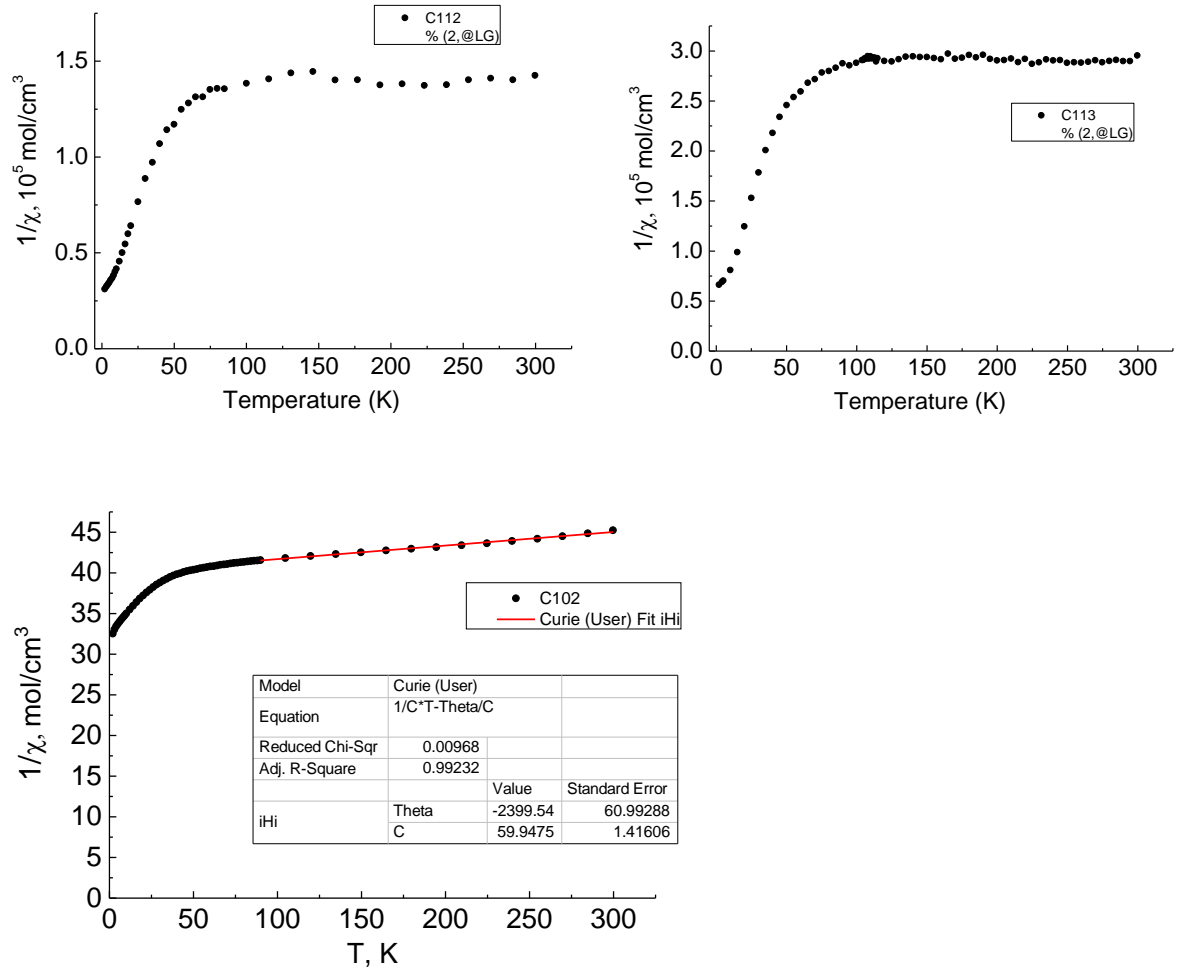


Figure S3. Temperature dependences of $1/\chi$ for $\text{Ni}_{5.80}\text{GaTe}_2$ (top left), $\text{Ni}_{9.39}\text{Ga}_2\text{S}_2$ (top right), and $\text{Ni}_{5.78}\text{InTe}_2$.

Table S1. Atomic coordinates and ADPs for $\text{Ni}_{5.80}\text{GaTe}_2$ based on the synchrotron single-crystal data.

Atom	Wyckoff site	x/a	y/b	z/c	S.O.F.	$U_{\text{iso}}, \text{\AA}^2$
Ni(1)	8g	1/2	1/2	0.41082(10)	1	0.0187(7)
Ni(2)	2b	1/2	1/2	1/2	1	0.0174(9)
Ni(3)	4e	1/2	1/2	0.1897(4)	0.397(16)	0.024(3)
Ga	2a	0	0	1/2	1	0.0184(8)
Te	4e	1/2	1/2	0.32036(6)	1	0.0190(6)