

Electronic Supplementary Information (ESI) available:

Modified Bridgman Growth and Characterization of a Novel Mid-infrared Nonlinear Optical Crystal: LiGa₃Te₅

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Fig. S1 Photograph of compact polycrystalline LGT.

Fig. S2 XRD pattern of polycrystalline LGT (up in blue) comparing with the calculated one (below in red).

Fig. S3 Specific heat of LGT crystal.

Table S1 Atomic Positions ($\times 10^4$) and Isotropic Displacement Factors ($\text{\AA}^2 \times 10^3$) for LGT

Table S2 Selected bond lengths (\AA) and angles (deg.) for LGT.

Fig. S1 Photograph of compact polycrystalline LGT.

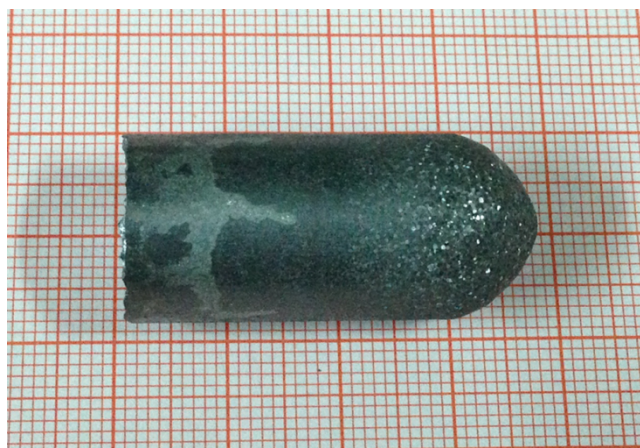


Fig. S2 XRD pattern of polycrystalline LGT (up in blue) comparing with the calculated one (below in red).

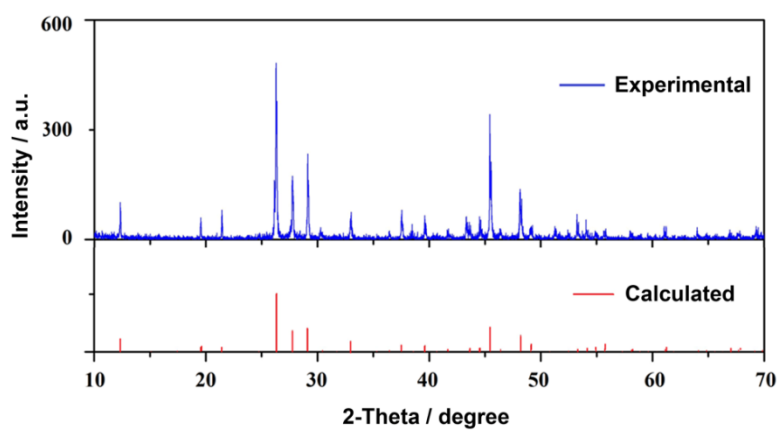


Fig. S3 Specific heat of LGT crystal.

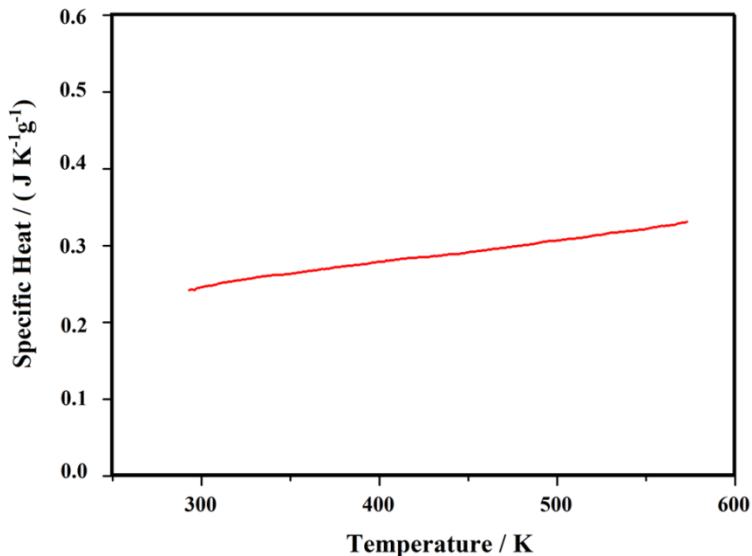


Table S1 Atomic Positions ($\times 10^4$) and Isotropic Displacement Factors ($\text{\AA}^2 \times 10^3$) for LGT

	x	y	z	$U(\text{eq})$
Te(5)	3893(1)	8590(1)	2875(1)	21(1)
Te(4)	6324(1)	8677(1)	4352(1)	15(1)
Te(3)	4149(1)	10000(1)	5000(1)	21(1)
Te(2)	6667(1)	11666(1)	3333(1)	20(1)
Te(1)	3333(1)	6667(1)	4954(1)	14(1)
Ga(1)	5842(1)	9981(1)	2477(1)	17(1)
Ga(2)	4446(1)	8574(1)	4288(1)	17(1)
Li(1)	4080(3)	10740(3)	3333(1)	34(1)
Li(2)	3333(2)	6667(2)	1667(1)	1(1)
Li(3)	3333(1)	6667(2)	1025(2)	1(2)

Table S2 Bond lengths (\AA) and angles (deg.) for LGT.

Te(5)-Ga(1)	2.5905(14)	Te(1)-Ga(2)	2.6536(13)
Te(5)-Ga(2)	2.6164(18)	Te(1)-Ga(2)#8	2.6536(13)
Te(5)-Li(3)#1	2.653(8)	Ga(1)-Te(4)#9	2.6524(18)
Te(5)-Li(1)	3.07(2)	Ga(1)-Te(4)#3	2.6623(15)
Te(5)-Li(2)	3.2521(13)	Li(1)-Te(5)#10	3.07(2)
Te(4)-Ga(2)	2.6249(15)	Li(1)-Te(3)#11	3.144(6)

Te(4)-Ga(1)#2	2.6524(18)	Li(1)-Te(2)#12	3.26(3)
Te(4)-Ga(1)#3	2.6622(15)	Li(2)-Li(3)#1	1.13(2)
Te(3)-Ga(2)#4	2.6091(13)	Li(2)-Te(5)#13	3.2520(13)
Te(3)-Ga(2)	2.6091(13)	Li(2)-Te(5)#1	3.2520(13)
Te(3)-Li(1)	3.144(6)	Li(2)-Te(5)#7	3.2521(13)
Te(3)-Li(1)#5	3.144(6)	Li(2)-Te(5)#8	3.2521(13)
Te(2)-Ga(1)	2.5803(13)	Li(2)-Te(5)#14	3.2521(13)
Te(2)-Ga(1)#3	2.5803(13)	Li(3)-Li(3)#1	2.26(4)
Te(2)-Li(1)#6	3.26(3)	Li(3)-Te(5)#13	2.653(8)
Te(2)-Li(1)	3.26(3)	Li(3)-Te(5)#1	2.653(8)
Te(1)-Ga(2)#7	2.6536(13)	Li(3)-Te(5)#14	2.653(8)
Ga(1)-Te(5)-Ga(2)	92.83(3)	Te(5)#10-Li(1)-Te(3)	85.9(4)
Ga(1)-Te(5)-Li(3)#1	110.3(2)	Te(5)-Li(1)-Te(3)	84.5(4)
Ga(2)-Te(5)-Li(3)#1	106.5(4)	Te(5)#10-Li(1)-Te(3)#11	84.5(4)
Ga(1)-Te(5)-Li(1)	77.3(6)	Te(5)-Li(1)-Te(3)#11	85.9(4)
Ga(2)-Te(5)-Li(1)	83.40(6)	Te(3)-Li(1)-Te(3)#11	162.3(13)
Li(3)#1-Te(5)-Li(1)	166.7(5)	Te(5)#10-Li(1)-Te(2)#12	85.16(17)
Ga(1)-Te(5)-Li(2)	100.91(3)	Te(5)-Li(1)-Te(2)#12	158.0(8)
Ga(2)-Te(5)-Li(2)	124.24(4)	Te(3)-Li(1)-Te(2)#12	108.9(6)
Li(3)#1-Te(5)-Li(2)	18.8(4)	Te(3)#11-Li(1)-Te(2)#12	85.0(4)
Li(1)-Te(5)-Li(2)	152.29(10)	Te(5)#10-Li(1)-Te(2)	158.0(8)
Ga(2)-Te(4)-Ga(1)#2	96.24(3)	Te(5)-Li(1)-Te(2)	85.16(17)
Ga(2)-Te(4)-Ga(1)#3	95.71(3)	Te(3)-Li(1)-Te(2)	85.0(4)
Ga(1)#2-Te(4)-Ga(1)#3	81.96(3)	Te(3)#11-Li(1)-Te(2)	108.9(6)
Ga(2)#4-Te(3)-Ga(2)	112.56(4)	Te(2)#12-Li(1)-Te(2)	78.9(8)
Ga(2)#4-Te(3)-Li(1)	111.2(7)	Li(3)#1-Li(2)-Te(5)#13	130.90(2)
Ga(2)-Te(3)-Li(1)	82.1(2)	Li(3)#1-Li(2)-Te(5)#1	130.90(2)

Ga(2)#4-Te(3)-Li(1)#5	82.1(2)	Te(5)#13-Li(2)-Te(5)#1	81.78(4)
Ga(2)-Te(3)-Li(1)#5	111.2(7)	Li(3)#1-Li(2)-Te(5)	49.10(2)
Li(1)-Te(3)-Li(1)#5	156.6(7)	Te(5)#13-Li(2)-Te(5)	113.59(3)
Ga(1)-Te(2)-Ga(1)#3	89.94(5)	Te(5)#1-Li(2)-Te(5)	159.571(17)
Ga(1)-Te(2)-Li(1)#6	120.5(3)	Li(3)#1-Li(2)-Te(5)#7	49.10(2)
Ga(1)#3-Te(2)-Li(1)#6	74.0(3)	Te(5)#13-Li(2)-Te(5)#7	159.573(17)
Ga(1)-Te(2)-Li(1)	74.0(3)	Te(5)#1-Li(2)-Te(5)#7	87.07(4)
Ga(1)#3-Te(2)-Li(1)	120.5(3)	Te(5)-Li(2)-Te(5)#7	81.78(4)
Li(1)#6-Te(2)-Li(1)	161.1(8)	Li(3)#1-Li(2)-Te(5)#8	49.10(2)
Ga(2)#7-Te(1)-Ga(2)	101.93(3)	Te(5)#13-Li(2)-Te(5)#8	87.07(4)
Ga(2)#7-Te(1)-Ga(2)#8	101.93(3)	Te(5)#1-Li(2)-Te(5)#8	113.59(3)
Ga(2)-Te(1)-Ga(2)#8	101.93(3)	Te(5)-Li(2)-Te(5)#8	81.78(4)
Te(2)-Ga(1)-Te(5)	112.04(4)	Te(5)#7-Li(2)-Te(5)#8	81.78(4)
Te(2)-Ga(1)-Te(4)#9	115.28(4)	Li(3)#1-Li(2)-Te(5)#14	130.90(2)
Te(5)-Ga(1)-Te(4)#9	104.42(3)	Te(5)#13-Li(2)-Te(5)#14	81.78(4)
Te(2)-Ga(1)-Te(4)#3	115.80(3)	Te(5)#1-Li(2)-Te(5)#14	81.78(4)
Te(5)-Ga(1)-Te(4)#3	110.27(3)	Te(5)-Li(2)-Te(5)#14	87.07(4)
Te(4)#9-Ga(1)-Te(4)#3	97.68(3)	Te(5)#7-Li(2)-Te(5)#14	113.59(3)
Te(3)-Ga(2)-Te(5)	106.33(4)	Te(5)#8-Li(2)-Te(5)#14	159.572(17)
Te(3)-Ga(2)-Te(4)	120.02(3)	Li(3)#1-Li(3)-Te(5)#13	112.1(4)
Te(5)-Ga(2)-Te(4)	110.32(3)	Li(3)#1-Li(3)-Te(5)#1	112.1(4)
Te(3)-Ga(2)-Te(1)	110.24(4)	Te(5)#13-Li(3)-Te(5)#1	106.7(5)
Te(5)-Ga(2)-Te(1)	113.65(4)	Li(3)#1-Li(3)-Te(5)#14	112.1(4)
Te(4)-Ga(2)-Te(1)	96.36(2)	Te(5)#13-Li(3)-Te(5)#14	106.7(5)
Te(5)#10-Li(1)-Te(5)	113.9(12)	Te(5)#1-Li(3)-Te(5)#14	106.7(5)
