

Supplementary Materials for

Li₃GaTe₄O₁₁: Small Ion-Driven Orientation of TeO_n Units in Tunnel-Structured Tellurite

Jingfang Zhou^{a§}, Pifu Gong^{d§}, Chang Gao^a, Mingjun Xia^{bc}, Jing Yu^a, Hongxia Zhang^a, and Qian Wu^{bc*}

^a Department of Chemistry, Tangshan Normal University, Hebei Tangshan 063000, China

^b Beijing Center for Crystal Research and Development, Key Laboratory of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China

^c School of Chemical Science, University of Chinese Academy of Sciences, Beijing 100049, China

^d Functional Crystals Lab, Key Laboratory of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100049, China

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1 、 Supplementary tables

Table S1. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2) of $\text{Li}_3\text{GaTe}_4\text{O}_{11}$.

Atom	Wyckoff	x/a	y/b	z/c	U(eq)/(\AA^2)	Uani
Te1	8f	0.83479(2)	0.33495(4)	0.32998(2)	0.01011(9)	1
Te2	8f	0.55607(2)	0.73783(5)	0.43787(3)	0.01616(9)	1
Ga1	4d	0.750000	0.750000	0.500000	0.00792(12)	1
O1	4e	0.500000	0.6261(8)	0.250000	0.0298(11)	1
O2	8f	0.56620(15)	1.0813(5)	0.4008(3)	0.0175(6)	1
O3	8f	0.64616(14)	0.6073(5)	0.4288(3)	0.0130(5)	1
O4	8f	0.77584(14)	0.4305(5)	0.4300(2)	0.0103(5)	1
O5	8f	0.76729(14)	0.4394(5)	0.1669(2)	0.0109(5)	1
O6	8f	0.88892(17)	0.6460(5)	0.3473(3)	0.0190(6)	1
Li1	8f	0.6717(5)	0.2439(14)	0.3832(8)	0.0229(16)	1
Li2	8f	0.4788(8)	1.232(3)	0.2709(14)	0.019(3)	0.5

Table S2. Bond lengths [\AA] of $\text{Li}_3\text{GaTe}_4\text{O}_{11}$.

Atom	Length/ \AA	Atom	Length/ \AA
Te1-O5	1.870(2)	Li1-O5	2.130(8)
Te1-O4	1.858(2)	Li1-O3	2.046(8)
Te1-O6	1.886(3)	Li1-O4	2.099(8)
Te2-O3	1.867(3)	Li1-O4	2.121(8)
Te2-O6	2.274(3)	Li1-O2	2.233(9)
Te2-O2	1.850(3)	Li1-O6	2.412(9)
Te2-O1	2.0265(13)	Li2-O2	1.936(14)
Ga1-O5	1.975(2)	Li2-O2	1.922(15)
Ga1-O5	1.975(2)	Li2-O1	2.108(14)
Ga1-O3	1.996(2)	Li2-O1	2.108(14)
Ga1-O3	1.996(2)	Li2-O6	2.170(15)
Ga1-O4	1.949(2)		

Ga1-O4-

1.949(2)

Table S3. Bond angles [°] of Li₃GaTe₄O₁₁.

Atom	Angle/°	Atom	Angle/°
O5-Te1-O6	91.29(12)	O4-Ga1-O4	180.0
O4-Te1-O5	96.44(11)	O5-Li1-O6	72.2(2)
O4-Te1-O6	97.25(12)	O5-Li1-O2	108.5(3)
O3-Te2-O6	91.96(11)	O3-Li1-O5	159.3(4)
O3-Te2-O1	91.50(9)	O3-Li1-O4	78.2(3)
O2-Te2-O3	100.11(12)	O3-Li1-O4	103.8(4)
O2-Te2-O6	85.34(12)	O3-Li1-O6	111.8(4)
O2-Te2-O1	96.76(14)	O3-Li1-O2	92.2(3)
O5-Ga1-O5	180.0	O4-Li1-O5	78.6(3)
O5-Ga1-O3	90.33(11)	O4-Li1-O5	81.8(3)
O5-Ga1-O3	89.67(11)	O4-Li1-O4	82.3(3)
O5-Ga1-O3	89.67(11)	O4-Li1-O6	142.6(4)
O5-Ga1-O3	90.33(11)	O4-Li1-O6	115.3(4)
O3-Ga1-O3	180.0	O4-Li1-O2	84.6(3)
O4-Ga1-O5	86.66(10)	O4-Li1-O2	161.4(4)
O4-Ga1-O5	93.34(10)	O2-Li1-O6	82.9(3)
O4-Ga1-O5	93.35(11)	O1-Li2-O6	116.2(7)
O4-Ga1-O5	86.65(11)	O2-Li2-O2	121.6(8)
O4-Ga1-O3	83.04(11)	O2-Li2-O1	108.8(6)
O4-Ga1-O3	83.04(11)	O2-Li2-O1	109.3(7)
O4-Ga1-O3	96.96(11)	O2-Li2-O6	103.4(6)
O4-Ga1-O3	96.96(11)	O2-Li2-O6	97.4(6)

Table S4. The bond valence sums (BVS) of Li₃GaTe₄O₁₁.

Element	BVS	Element	BVS
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Te1	4.07	O1	-1.91
Te2	3.94	O2	-1.82
Ga1	3.06	O3	-2.03
Li1	0.96	O4	-2.20
Li2	0.86	O5	-2.06
		O6	-1.86

2、Supplementary figures

Figure S1. The PXRD pattern of $\text{Li}_3\text{GaTe}_4\text{O}_{11}$.

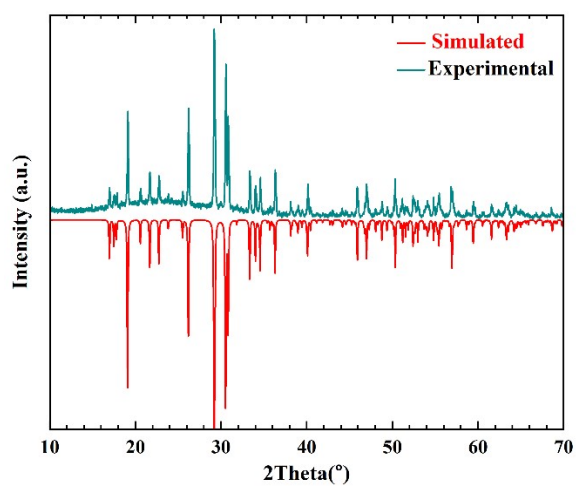


Figure S2. The PXRD patterns before and after thermal test.

