Investigation of the homogeneity of BGO single crystal, a promising X–ray diffraction standard

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Supplementary materials

Table S1 The result of single-crystal x-ray diffraction analysis for BGO sample **1** at the temperature of 300 K

Crystal data	
Chemical formula	$Bi_4Ge_3O_{12}$
Mr	1245.69
Crystal system, space group	Cubic, *I*-43*d*
Temperature (K)	300
a (Å)	10.5193(1)
V (Å3)	1164.02(3)
Z	4
Radiation type	MoKα
μ (mm^{-1})	67.95
Crystal size (mm)	0.05 × 0.05 × 0.05
Data collection	
Diffractometer	Bruker D8 VENTURE
Absorption correction	Multi-scan Bruker SADABS2012/1
T_{min}, T_{max}	0.374, 0.746
No. of measured, independent and observed [I > 2σ(I)] reflections	3508, 327, 324
R_{int}	0.037
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.733
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.014, 0.032, 1.22
No. of reflections	327
No. of parameters	16
$\Delta\rho_{max}$, $\Delta\rho_{min}$ ($eÅ^{-3}$)	1.11, −1.29
Absolute structure	Flack x determined using 136 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.049 (11)

The coordinates of the atoms (×104) and the thermal parameter U_{eq} (Å2×103)

Atom	x	y	z	U_{eq}
Bi01	3375.3(2)	3375.3(2)	3375.3(2)	7.05(14)
Ge02	5000	2500	6250	5.6(2)
O003	3765(5)	3195(5)	5377(4)	12.0(8)

Computer programs: Bruker *APEX3* V2018.7-2, *SAINT* V8.38A, SHELXT 2018/2, SHELXL 2018/3, Olex2 v.1.5 (Dolomanov et al., 2019).

Table S2 Dynamics of BGO crystal **1** structure parameters in the temperature range 140-480 K. The designations are given according to Fig. S1

140-300 K					
T, K	140	180	220	260	300
Deposition number	2428455	2428456	2428457	2428458	2388565
a, Å	10.5123(3)	10.5145(2)	10.5129(4)	10.5169(1)	10.5193(1)
Bi1-O5, Å	2.606(5)	2.610(5)	2.610(5)	2.610(5)	2.613(5)
Bi1-O6, Å	2.157(5)	2.155(5)	2.155(5)	2.153(5)	2.154(4)
Ge-O, Å	1.750(5)	1.751(5)	1.750(5)	1.751(5)	1.751(5)
O6-Bi1-O5, °	70.5(2)	70.5(2)	70.6(2)	70.4(2)	70.52(19)
O1-Bi1-O6, °	84.27(8)	84.24(7)	84.23(7)	84.25(7)	84.23(7)
O3-Bi1-O5, °	114.03(9)	114.05(8)	114.03(9)	114.01(9)	114.00(8)
O3-Bi1-O6, °	154.12(19)	154.10(18)	154.11(19)	154.24(19)	154.23(18)
O2-Bi1-O4, °	85.1(2)	85.1(2)	85.1(2)	85.3(2)	85.2(2)
O8-Ge-O6, °	117.0(3)	116.8(3)	116.9(3)	116.8(3)	116.7(3)
O7-Ge-O6, °	105.82(15)	105.91(14)	105.91(15)	105.95(14)	105.96(13)
Bi1-O6- Bi2, °	108.8(2)	108.76(19)	108.7(2)	108.8(2)	108.71(19)
Bi1-O6- Ge, °	133.5(3)	133.6(3)	133.6(3)	133.7(3)	133.7(2)
Bi2-O6- Ge, °	114.1(2)	114.0(2)	114.0(2)	114.0(2)	114.0(2)
U_{iso} (Bi), Å^2×10^3	3.92(15)	4.48(15)	5.24(15)	6.23(15)	7.05(14)
U_{iso} (Ge), Å^2×10^3	3.1(3)	3.5(2)	4.2(3)	4.9(2)	5.6(2)
U_{iso} (O), Å^2×10^3	6.4(8)	6.9(8)	9.1(8)	9.8(8)	12.0(8)
V(BiO_6), Å3	15.19(4)	15.19(3)	15.20(3)	15.19(3)	15.22(3)
V(GeO_4), Å^3	2.71(3)	2.72(2)	2.72(2)	2.72(2)	2.72(2)

320-480 K						
T, K	320	360	400	440	480	
Deposition number	2428450	2428451	2428453	2428454	2428452	$\|\Delta^*\|/\sigma_{max}$
a, Å	10.5207(1)	10.5236(1)	10.5236(2)	10.5281(2)	10.5321(1)	49.5
Bi1-O5, Å	2.616(5)	2.617(4)	2.619(4)	2.619(5)	2.617(5)	2.6
Bi1-O6, Å	2.152(5)	2.150(4)	2.152(4)	2.153(5)	2.153(5)	1.4
Ge-O, Å	1.751(5)	1.753(4)	1.750(4)	1.749(5)	1.753(5)	0.8
O6-Bi1-O5, °	70.5(2)	70.51(18)	70.61(18)	70.6(2)	70.4(2)	1.0
O1-Bi1-O6, °	84.19(8)	84.19(7)	84.17(7)	84.19(7)	84.24(8)	1.2
O3-Bi1-O5, °	114.01(9)	114.04(8)	113.98(8)	113.93(9)	113.94(9)	1.3
O3-Bi1-O6, °	154.2(2)	154.18(17)	154.27(18)	154.4(2)	154.5(2)	2.0
O2-Bi1-O4, °	85.2(2)	85.20(19)	85.2(2)	85.3(2)	85.5(2)	2.0

O8-Ge-O6, °	116.5(3)	116.5(3)	116.4(3)	116.5(3)	116.6(3)	2.0
O7-Ge-O6, °	106.07(14)	106.09(13)	106.10(13)	106.09(14)	106.05(15)	1.9
Bi1-O6- Bi2, °	108.7(2)	108.72(18)	108.60(17)	108.6(2)	108.8(2)	1.0
Bi1-O6- Ge, °	133.9(3)	133.9(2)	133.9(2)	134.0(3)	133.8(3)	1.7
Bi2-O6- Ge, °	113.9(2)	113.8(2)	113.98(8)	113.9(2)	114.0(2)	1.5
U_{iso} (Bi), Å^2×10^3	7.46(15)	8.41(14)	9.29(14)	10.29(16)	11.30(16)	46.1
U_{iso} (Ge), Å^2×10^3	5.8(2)	6.5(2)	7.0(2)	7.9(2)	8.7(3)	18.7
U_{iso} (O), Å^2×10^3	12.3(9)	13.9(8)	15.6(8)	17.5(9)	18.6(10)	12.2
V(BiO_6), Å3	15.23(3)	15.21(3)	15.26(3)	15.29(3)	15.29(4)	2.7
V(GeO_4), Å^3	2.72(3)	2.73(2)	2.72(2)	2.72(2)	2.73(3)	0.7

*Δ=value$_{max}$-value$_{min}$

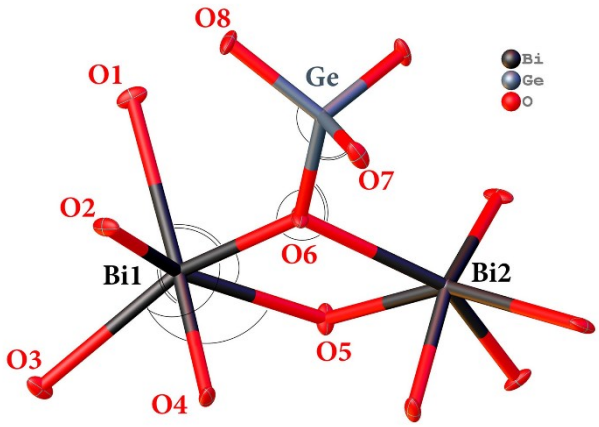

Figure S1 A fragment of the BGO structure with the indicated designations of atoms. All same element atoms are linked-connected.

Table S3 Determination of the crystals **9** and **10** UCP during the temperature experiment. In the first part of the table, the coordinates of the (12 4 4)$_{Si}$ reflection with reference angular positions $2\theta_{K\alpha1}$ = 120.070° and $2\theta_{K\alpha2}$ = 121.283° in 2 experiments (according to the crystals numbers) and the results of calculating the angular pixel size are given. The error values are similar to those shown in the Table 1 and are given only for UCP

			Si		
N	$X_{K\alpha1}$, pix.	$Y_{K\alpha1}$, pix.	$X_{K\alpha2}$, pix.	$Y_{K\alpha2}$, pix.	g, °
9	389.773	504.500	406.763	504.557	0.07092
10	389.554	502.822	406.657	502.925	0.07140
			BGO, crystal **9**		
T	$X_{K\alpha1}$, pix.	$Y_{K\alpha1}$, pix.	$2\theta_{K\alpha1}$, °	*d*, Å	*a*, Å
500	389.983	513.175	120.100	0.40932	10.5315(5)
480	390.275	513.749	120.121	0.40927	10.5304(5)
460	390.578	513.271	120.143	0.40923	10.5293(5)
440	391.024	511.771	120.174	0.40917	10.5276(5)
420	391.378	508.887	120.199	0.40911	10.5262(5)
400	391.649	505.673	120.219	0.40907	10.5252(5)

380	392.003	503.178	120.244	0.40902	10.5239(5)
360	392.423	501.903	120.274	0.40896	10.5223(5)
340	392.741	500.828	120.296	0.40892	10.5212(5)
320	393.128	499.889	120.324	0.40886	10.5197(5)
300	393.506	499.067	120.350	0.40880	10.5183(5)
280	393.839	498.255	120.374	0.40876	10.5171(5)
260	394.213	497.585	120.400	0.40870	10.5157(5)
240	394.518	496.860	120.422	0.40866	10.5145(5)
220	394.846	496.110	120.445	0.40861	10.5133(5)
200	395.197	495.432	120.470	0.40856	10.5120(5)
180	395.518	494.819	120.493	0.40851	10.5108(5)
160	395.795	494.251	120.513	0.40847	10.5098(5)
140	396.067	493.721	120.532	0.40843	10.5088(5)
120	396.320	493.272	120.550	0.40840	10.5078(5)
100	396.484	492.765	120.562	0.40837	10.5072(5)

BGO, crystal **10**

T	$X_{K\alpha1}$, pix.	$Y_{K\alpha1}$, pix.	$2\theta_{K\alpha1}$, °	*d*, Å	*a*, Å
430	391.353	511.740	120.145	0.40923	10.5271(5)
410	391.753	511.752	120.183	0.40915	10.5256(5)
390	392.212	510.703	120.211	0.40909	10.5239(5)
370	392.510	509.477	120.244	0.40902	10.5228(5)
350	392.827	509.150	120.265	0.40898	10.5216(5)
330	393.203	508.700	120.288	0.40893	10.5202(5)
310	393.570	508.377	120.315	0.40888	10.5188(5)
300	393.769	508.217	120.341	0.40882	10.5180(5)
280	394.021	507.895	120.355	0.40879	10.5171(5)
260	394.471	507.655	120.373	0.40876	10.5154(5)
240	394.784	507.392	120.405	0.40869	10.5142(5)
220	395.146	507.278	120.428	0.40865	10.5129(5)
200	395.508	507.057	120.454	0.40859	10.5115(5)
180	395.734	506.802	120.479	0.40854	10.5107(5)
160	396.058	506.523	120.496	0.40851	10.5094(5)
140	396.340	506.238	120.519	0.40846	10.5084(5)
120	396.503	505.732	120.539	0.40842	10.5079(5)
100	396.701	505.707	120.551	0.40840	10.5070(5)