Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Hydrothermal synthesis and crystal structure of a novel double-perovskite-type bismuth oxide with 3:1 ordering at the B-site

Khandaker Monower Hossain[a], Md Saiduzzaman[b], Nobuhiro Kumada[a*], Takahiro Takei[a], Hisanori Yamane[c]

[a]Center for Crystal Science and Technology, University of Yamanashi, 7-32 Miyamae-cho, Kofu 400-8511, Japan

[b]Department of Materials Science and Engineering, Khulna University of Engineering & Technology (KUET), Khulna-9203, Bangladesh

[c]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

Corresponding author email: kumada@yamanashi.ac.jp

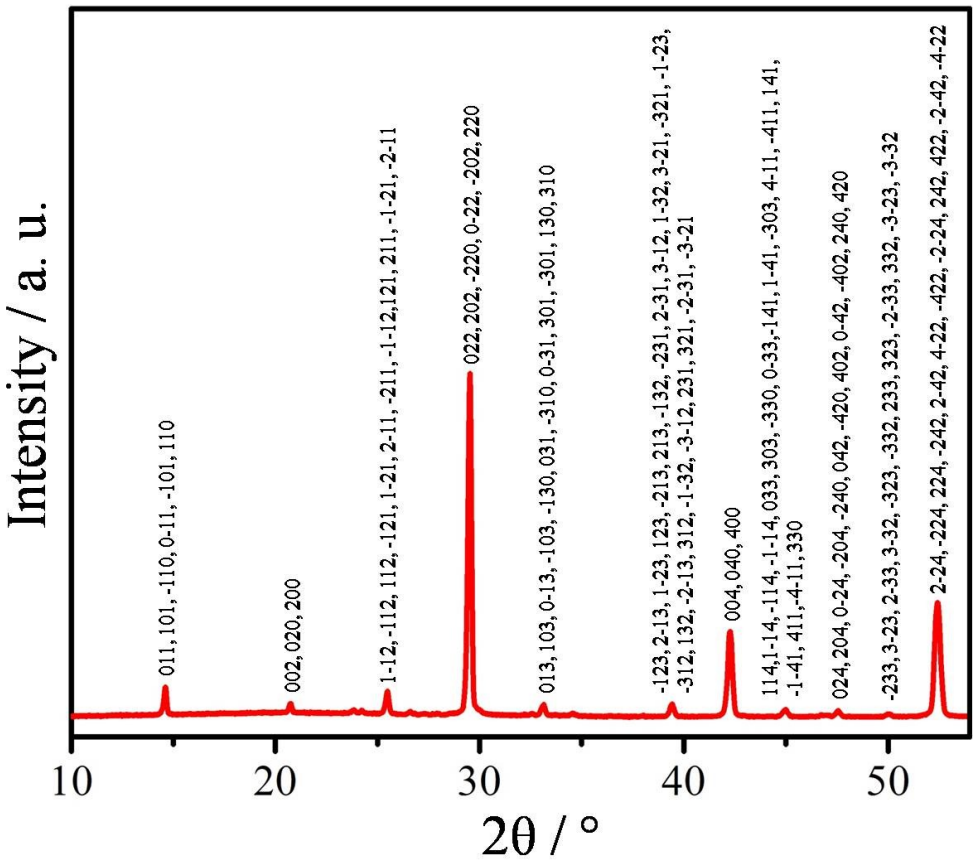

Fig. S1. XRD pattern of hydrothermally prepared sample at 240 °C.

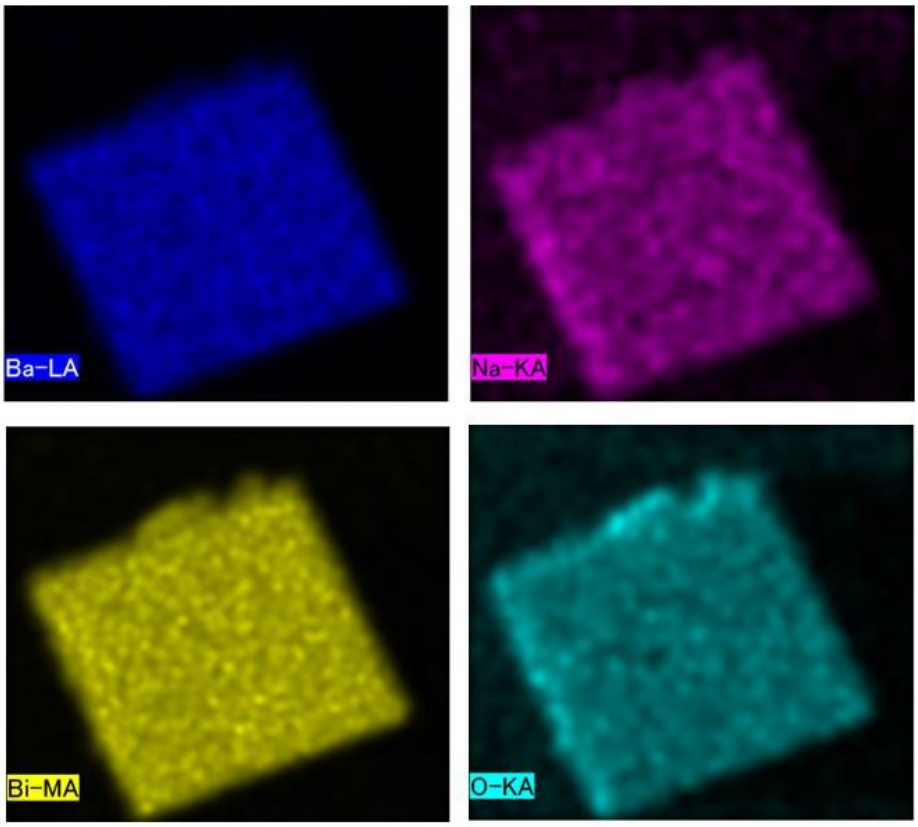

Fig. S2. EDS elemental mapping of hydrothermally synthesized $Ba_4Bi_3NaO_{12}$.

Table S1. Single-crystal data of $Ba_4Bi_3NaO_{12}$

Chemical formula	$Ba_4Bi_3NaO_{12}$
Formula weight (g mol^{-1})	1391.29
Crystal color	Black
Temperature, T (K)	298
Crystal system	Triclinic
Space group	*P*-1 (No. 2)
Unit-cell dimensions	
a (Å)	8.5415 (2)
b (Å)	8.5421 (2)
c (Å)	8.5441 (2)
α	89.996 (1)°
β	89.995 (1)°
γ	90.016 (1)°
Cell Volume, *V* ($Å^3$)	623.40 (3)
Z	2
Calculated density, D_{cal} (g cm^{-3})	7.412
Radiation wavelength, λ (Å)	0.71073
Absorption coefficient, m (mm^{-1})	54.702
F_{000}	1160
N_{ref}	2870
Goodness-of-fit on F^2, S	1.167
R_1, wR_2 (all data)	0.0202, 0.0476

Table S2. Structural parameters of $Ba_4Bi_3NaO_{12}$

Atom	Site	x	y	z	Occupancy	U_{eq}
Bi1	1g	0	0.5	0.5	0.104 (2)	0.0121 (8)
Na1	1g	0	0.5	0.5	0.896 (2)	0.0121 (8)
Bi2	1d	0.5	0	0	0.103 (2)	0.0150 (9)
Na2	1d	0.5	0	0	0.897 (2)	0.0150 (9)
Bi3	1b	0	0	0.5	0.9602 (15)	0.00825 (14)
Na3	1b	0	0	0.5	0.0398 (15)	0.00825 (14)
Bi4	1e	0.5	0.5	0	0.9568 (15)	0.00839 (14)
Na4	1e	0.5	0.5	0	0.0432 (15)	0.00839 (14)
Bi5	1f	0.5	0	0.5	1.0	0.0100 (4)
Bi6	1c	0	0.5	0	1.0	0.0102 (4)
Bi7	1h	0.5	0.5	0.5	0.9369 (18)	0.0101 (4)
Na7	1h	0.5	0.5	0.5	0.0631 (18)	0.0101 (4)
Bi8	1a	0	0	0	0.9396 (18)	0.0106 (4)
Na8	1a	0	0	0	0.0604 (18)	0.0106 (4)
Ba1	2i	0.25113 (7)	0.75094 (5)	0.25029 (6)	1.0	0.0271 (4)
Ba2	2i	0.24917 (7)	0.25072 (5)	0.24890 (6)	1.0	0.0270 (4)
Ba3	2i	0.24968(6)	0.74945 (4)	0.75019 (5)	1.0	0.0118 (3)
Ba4	2i	0.25001 (6)	0.24939 (4)	0.74878 (5)	1.0	0.0115 (3)
O1	2i	0.5128 (7)	0.9789 (6)	0.2684 (7)	1.0	0.0218 (12)
O2	2i	-0.0108 (7)	0.4802 (6)	0.2316 (7)	1.0	0.0203 (12)
O3	2i	-0.0035 (7)	0.2324 (4)	0.5279 (5)	1.0	0.0165 (8)
O4	2i	0.5037 (7)	0.7328 (4)	0.9733 (5)	1.0	0.0160 (8)
O5	2i	0.2661 (10)	0.4963 (9)	0.5111 (9)	1.0	0.0372 (18)
O6	2i	0.2322 (8)	-0.0027 (7)	-0.0173 (7)	1.0	0.0238 (14)
O7	2i	0.2499 (8)	1.0035 (7)	0.4810 (7)	1.0	0.0282 (15)
O8	2i	0.2474 (9)	0.5035 (8)	0.0106 (9)	1.0	0.042 (2)
O9	2i	1.0107 (7)	0.0248 (7)	0.2495 (7)	1.0	0.0242 (12)
O10	2i	0.4867 (7)	0.5235 (6)	0.2490 (7)	1.0	0.0225 (12)
O11	2i	0.5029 (8)	0.2495 (7)	0.4683 (5)	1.0	0.0191 (8)
O12	2i	-0.0037 (8)	0.7492 (7)	0.0291 (5)	1.0	0.0166 (8)

Table S3. Selected interatomic distance (Å) for $Ba_4Bi_3NaO_{12}$

Ba1-O1	2.968 (6)	Ba2-O2	2.966 (6)
Ba1-O3	2.843 (6)	Ba2-O4	2.842 (6)
Ba1-O5	3.117 (8)	Ba2-O5	3.073 (8)
Ba1-O6	3.112 (7)	Ba2-O6	3.143 (7)
Ba1-O7	2.922 (6)	Ba2-O7	2.897 (6)
Ba1-O8	2.943 (8)	Ba2-O8	2.968 (8)
Ba1-O9	3.113 (7)	Ba2-O9	2.806 (7)
Ba1-O10	2.797 (6)	Ba2-O10	3.089 (6)
Ba1-O12	2.883 (6)	Ba2-O11	2.866 (6)
Mean	2.966	**Mean**	2.961

Ba3-O1	3.086 (6)	Ba4-O1	2.816 (6)
Ba3-O2	2.834 (6)	Ba4-O2	3.089 (6)
Ba3-O4	2.892 (6)	Ba4-O3	2.876 (6)
Ba3-O5	2.978 (8)	Ba4-O5	2.931 (8)
Ba3-O6	2.907 (6)	Ba4-O6	2.942 (6)
Ba3-O8	3.060 (8)	Ba4-O7	3.106 (6)
Ba3-O9	2.944 (6)	Ba4-O8	3.117 (8)
Ba3-O11	2.820 (6)	Ba4-O10	2.970 (6)
Mean	2.940	Ba4-O12	2.833 (6)
		Mean	2.964

Bi1/Na1-O2	2.301 (6)	Bi2/Na2-O1	2.303 (6)
Bi1/Na1-O2	2.301 (6)	Bi2/Na2-O1	2.303 (6)
Bi1/Na1-O3	2.298 (4)	Bi2/Na2-O4	2.294 (4)
Bi1/Na1-O3	2.298 (4)	Bi2/ Na2-O4	2.294 (4)
Bi1/Na1-O5	2.275 (9)	Bi2/Na2-O6	2.292 (7)
Bi1/Na1-O5	2.275 (9)	Bi2/Na2-O6	2.292 (7)
Mean	2.291	**Mean**	2.296

Bi3/Na3-O3	2.000 (4)	Bi4/Na4-O4	2.002 (4)
Bi3/Na3-O3	2.000 (4)	Bi4/Na4-O4	2.002 (4)
Bi3/Na3-O7	2.141 (7)	Bi4/Na4-O8	2.160 (8)
Bi3/Na3-O7	2.141 (7)	Bi4/Na4-O8	2.160 (8)
Bi3/Na3-O9	2.153 (6)	Bi4/Na4-O10	2.140 (6)
Bi3/Na3-O9	2.153 (6)	Bi4/Na4-O10	2.140 (6)
Mean	2.098	**Mean**	2.100

Bi5-O1	1.990 (6)	Bi6-O2	1.988 (6)
Bi5-O1	1.990 (6)	Bi6-O2	1.988 (6)
Bi5-O7	2.143 (7)	Bi6-O8	2.115 (8)
Bi5-O7	2.143 (7)	Bi6-O8	2.115 (8)
Bi5-O11	2.149 (6)	Bi6-O12	2.143 (6)
Bi5-O11	2.149 (6)	Bi6-O12	2.143 (6)
Mean	2.094	**Mean**	2.082

Bi7/Na7-O5	2.000 (9)	Bi8/Na8-O6	1.989 (7)
Bi7/Na7-O5	2.000 (9)	Bi8/Na8-O6	1.989 (7)
Bi7/Na7-O10	2.157 (6)	Bi8/Na8-O9	2.144 (6)
Bi7/Na7-O10	2.157 (6)	Bi8/Na8-O9	2.144 (6)
Bi7/Na7-O11	2.157 (6)	Bi8/Na8-O12	2.157 (6)
Bi7/Na7-O11	2.157 (6)	Bi8/Na8-O12	2.157 (6)
Mean	2.104	**Mean**	2.096

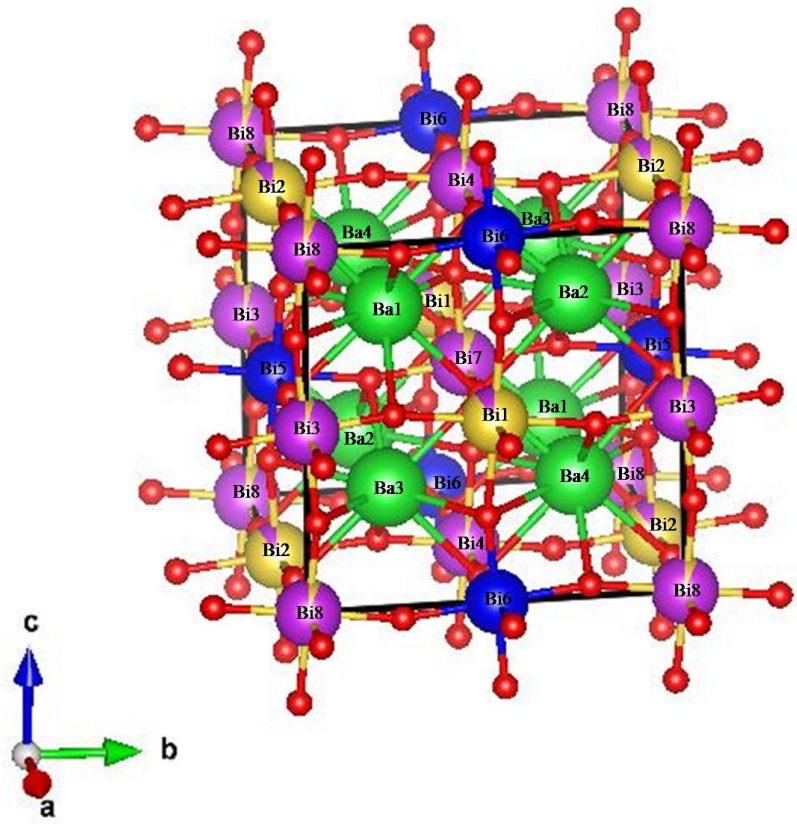

Fig. S3. Crystal structure of hydrothermally synthesized $Ba_4Bi_3NaO_{12}$ at 240°C.

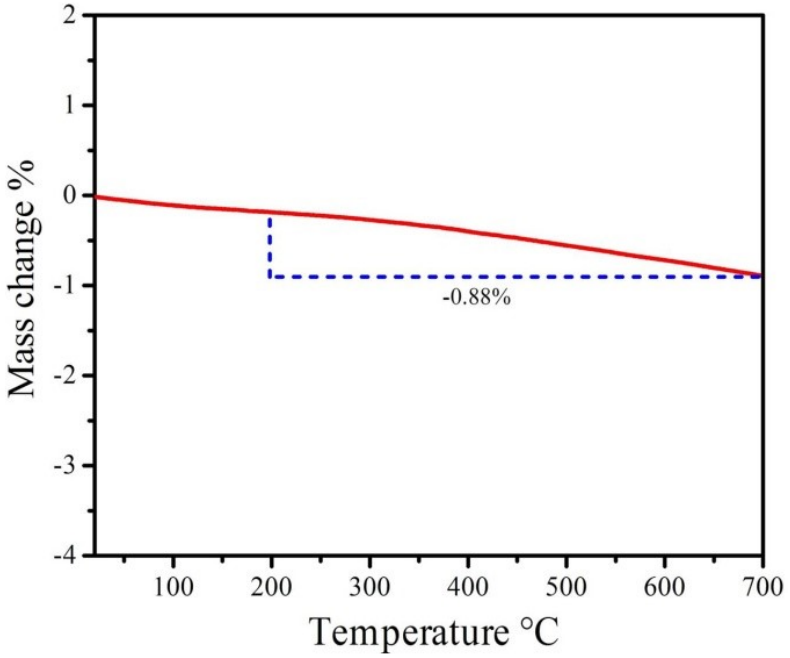

Fig. S4. TG curve of hydrothermally prepared $Ba_4Bi_3NaO_{12}$ at 240°C.

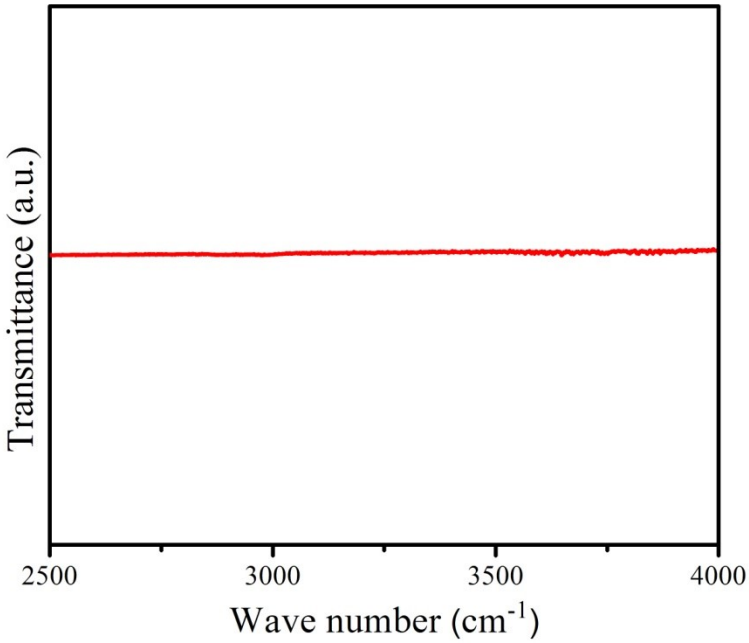

Fig. S5. FT-IR spectrum of hydrothermally prepared $Ba_4Bi_3NaO_{12}$ at 240°C.

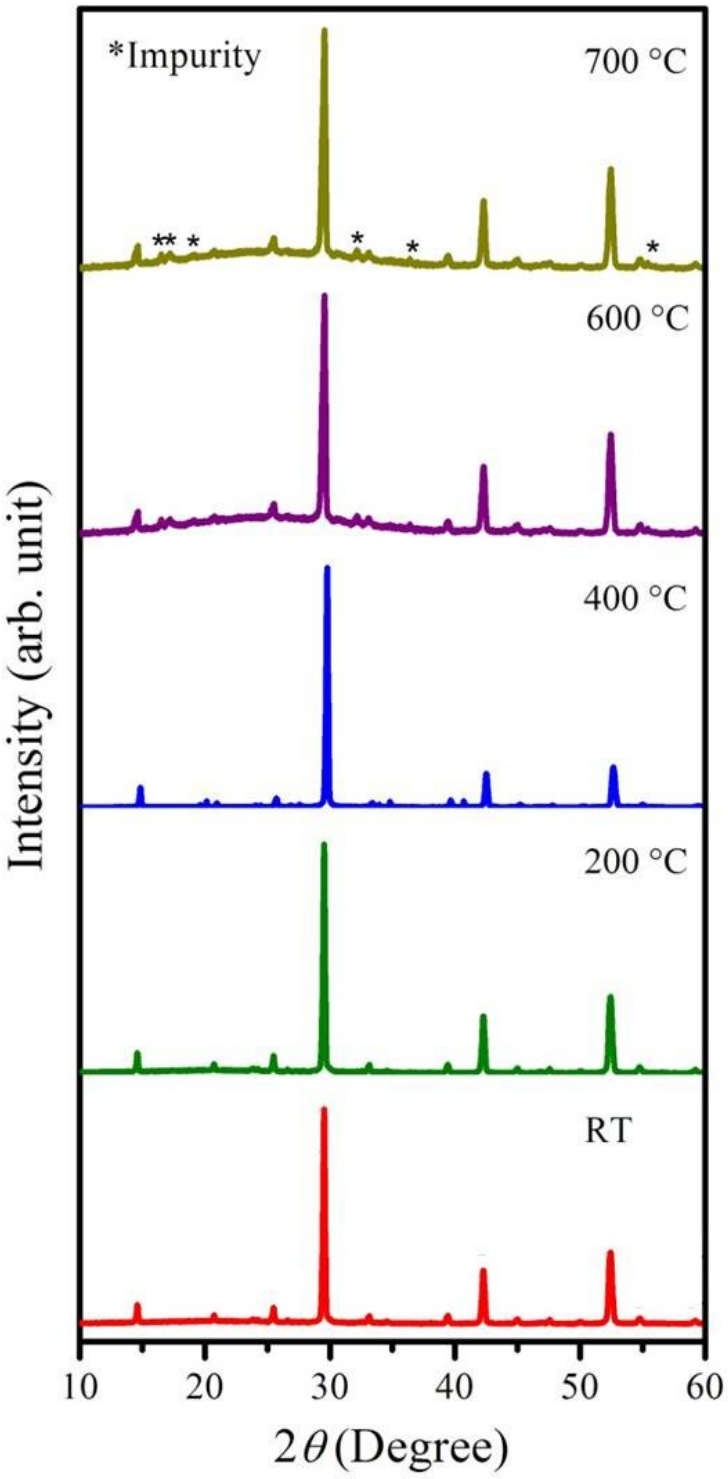

Fig. S6. XRD patterns of $Ba_4Bi_3NaO_{12}$ heated at different temperatures from room temperature to 700 °C.

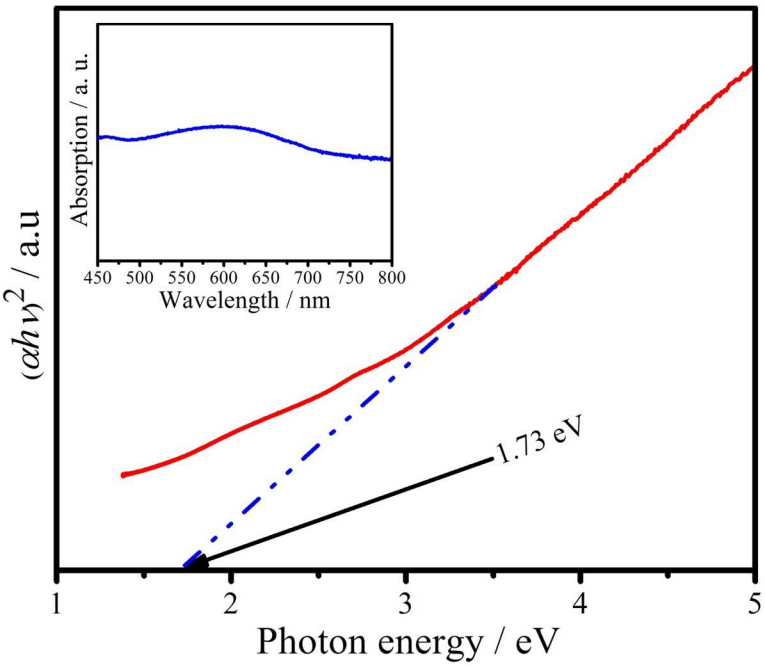

Fig. S7. Tauc plot for the estimation of the band gap of $Ba_4Bi_3NaO_{12}$. The inset shows the absorption spectrum.

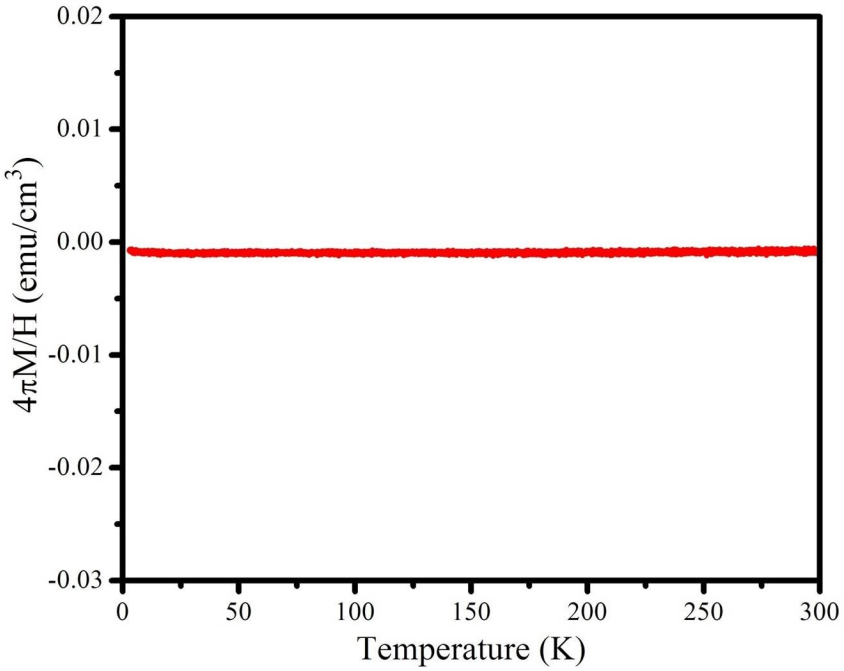

Fig. S8. DC magnetic susceptibility of hydrothermally synthesized $Ba_4Bi_3NaO_{12}$.

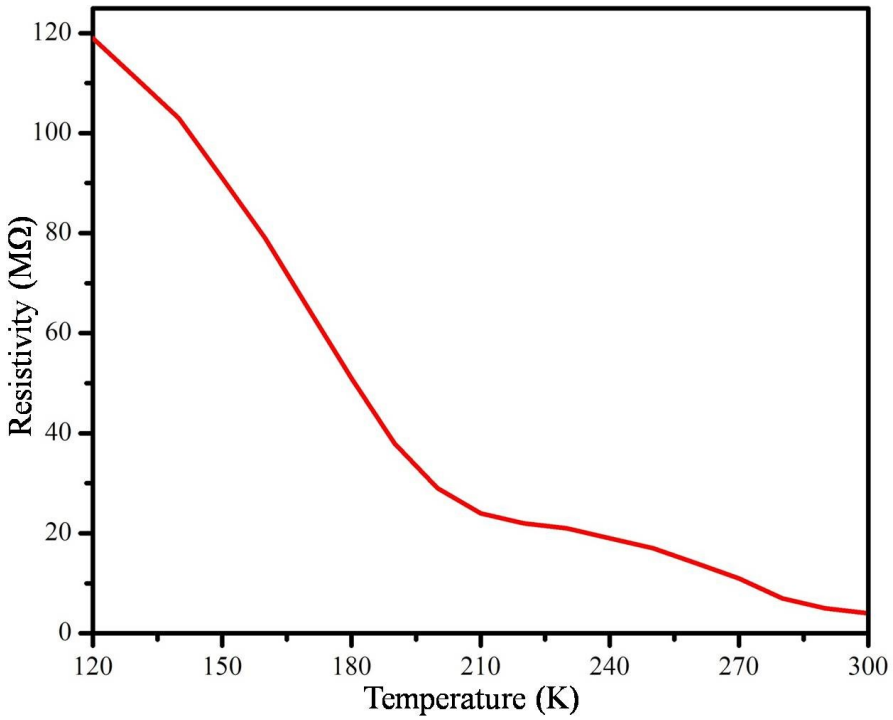

Fig. S9. Temperature-dependent electrical resistivity of hydrothermally prepared $Ba_4Bi_3NaO_{12}$.