Available online at www.elixirpublishers.com (Elixir International Journal)

Crystal Growth

Elixir Crystal Growth. 32 (2011) 2041-2045

ISSN: 2229-712X

Synthesis, crystal structure determination and ionic properties of novel Bi $Ca_{0.5}Mg_{0.5}$ $O_{2.5}$ via X- ray powder diffraction data

Parashuram Mishra
Department of Chemistry, Tribhuvan University,Nepal.

ARTICLE INFO

Article history:
Received: 4 February 2011;
Received in revised form:
25 February 2011;
Accepted: 2 March 2011;

Keywords
Crystal structures,
X-ray powder diffraction,
Metal oxide,
AFM technique,
Morphology.

ABSTRACT
The crystal structure of Bi $Mg_{0.5}Mg_{0.5}$ $O_{2.5}$ has been determined by direct methods using integrated intensities of X-ray powder diffraction data and subsequently refined with the Rietveld technique. The titled compound was prepared from mixture of $Bi_2(CO_3)_3$, $MgCO_3$ and $CaCO_3$ by care full thermal decomposition at 1000°C. The metallic oxide adopts orthorhombic symmetry space group P_{NMA} with unit cell parameters A = 23.104910Å, b = 12.618820 Å, c = 3.033075Å, β = 90°, V = 884.31Å and Z = 2. D : 1.869 M_{11} = 10, F_{11} = 5. The final reliability indices calculated from the Rietveld refinement were Rwp = 0.0517, R_p = 0.022 and R_p = 0.082. The structure factors F_0 = 3073 and F_c = 3163. The morphology of the crystal has been determined by Atomic Force Microscope technique and by SEM too. The DC conductivity has been determined and showed ionic properties at different temperature.

Introduction

Oxide ion conductors have been a subject of extensive study due to their potential application in fuel cells, oxygen sensors, oxygen pumps, dense membranes for oxygen separation and catalysis. Over the past decade, many efforts have been made to develop new materials exhibiting high oxide ion mobility at ambient temperature. In addition to the improvements of the existing materials, new class of conductors in which in which the structure plays an important role have been proposed. The present paper is part of systematic investigation on the crystal structure in the system Bi_2O_3–CaO–MgO. The triple oxides belonging to this system are of interest in both materials science and earth science and their phase relations have been studied [1]. Single-crystal X-ray diffraction is undoubtedly the most powerful and widely used technique for elucidating the structures of organic and metal-organic compounds and inorganic complexes, an intrinsic limitation of this technique is the requirement to prepare single crystal of sufficient size, quality, and stability, which are not always met for all compounds using the chosen crystal growth conditions and within a reasonable time-scale. In such circumstances, X-ray powder diffraction can be an alternate route for structural analysis. Compared with other methods, such as scanning electron microscopy, and transmission electron microscopy, atomic force microscopy has the advantage to understand the change in morphological condition with high-resolution.

Although much work has been done on physical properties of solid metal oxide [2], there are still many unanswered questions about conductivity mechanism, and structure of these materials. The present paper reports the results of d.c. and a.c. conductivity measurements in $BiCa_{0.5}Mg_{0.5}$ $O_{2.5}$. The temperature dependent electrical conductivity data have been analysed with the objective of understanding the conduction mechanism. In this work a novel oxide $BiCa_{0.5}Mg_{0.5}$ $O_{2.5}$which also belongs to the family of $A_{0.5}Mg_{0.5}Ca_{0.5}$ was found through the study of Bi_2O_3–CaO–MgO ternary system. The crystal structure of $BiCa_{0.5}Mg_{0.5}$ $O_{2.5}$was determined by the Rietveld refinement method from X-ray powder diffraction data at room temperature.

Experimental Section

All chemicals used were analytical grade. A polycrystalline sample of $BiCa_{0.5}Mg_{0.5}$ $O_{2.5}$ was synthesized by a standard solid state reaction using a mixture of high purity reagents of $MgCO_3$, $CaCO_3$ and $Bi_2(CO_3)_3$ as the starting materials in the molar ratio of 2 : 1 : 1. The mixture was ground carefully, homogenized thoroughly with methanol (99%) in an agate mortar and then packed into an alumina crucible and calcined at 1000°C in air for 30h with several intermediate grindings.

Finally the product was pressed into pallets and sintered at 100 K/h. Powder X-ray diffraction (XRD) data were collected at room temperature in the angular range of 2θ $=10^0$-70^0 with scan step width of 0.02° and a fixed containing time of 15 s using Philips powder diffractometer with graphite monochromatic CuK_α radiation. The powder was rotated during the data collection to minimize preferred Orientation effect if any. The program TREOR in CRYSFIRE [6-7] was used to index the powder pattern which give orthorhombic cell system.SIRPOW92 was used to locate the positional parameters of constituent atoms. The full pattern is fitting and peak decomposition in the space group PNMA using check cell program. The structural parameters were refined by the Reitveld method using the GSAS program which gave R_{wp} = 0.0517, R_p= 0.022, R_p = 0.082. The density is determined by Archimedes principle. The morphology of titled compound was determined using AFM (Nanoscope III, Digital Instruments, Santa Barbara).

Results and Discussion

The synthesized $BiO_{2.5}Ca_{0.5}Mg_{0.5}$ compound is shinning white in colour, in contrast to the pale cream observed for bismuth oxide. XRD suggested that the product was single phase with the orthorhombic (Pmmm) super structure exhibited by $Bi_2Ca_2Mg_2O_{10}$. The synthesis conditions ultimately form stable Bi(III) rather than higher valent ions. Infra-red spectroscopy, revealed bands of metal carbonates (Calcium and magnesium) in

Tele:
E-mail addresses: prmmishra@rediffmail.com

the starting materials in the range of 1510-700cm^{-1} are disappeared in the solid product. Indexing Bragg reflections in the XRD data indicated that $BiO_{2.5}Ca.Mg$ crystalline in the orthorhombic system. The figure of merit for assessing the quality of the solution are M_{11} = 10, F_{11} = 5 and Av. Eps = 0.0000673 crystallographic and experimental parameters are given in Table 1, final positional bond lengths, bond angles dihedral angles and torsion angles are given in table 2, and their fraction coordinates are discussed in table 4. We found that $BiO_{2.5}Ca_{0.5}Mg_{0.5}$ displays a spiral chain structure viewed along the c-axis [3-5].

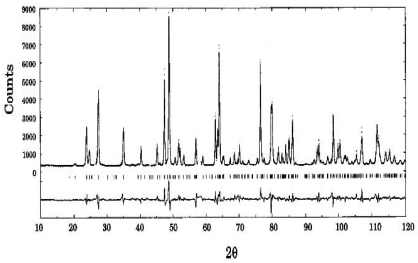

Fig.1: Observed, calculated and difference X-ray diffraction pattern of $BiO_{2.5}Ca_{0.5}Mg_{0.5}$.

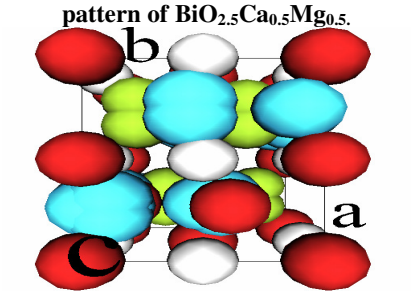

Fig.2.Closed-packed structure of oxide.

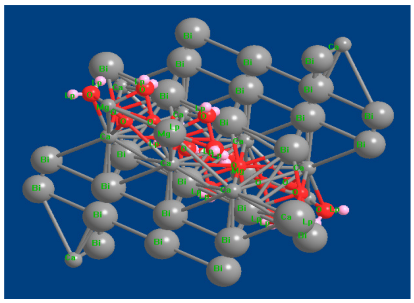

Fig3: Three dimensional structure of $BiCa_{0.5}Mg_{0.5}O_{2.5}$

The observed, difference and calculated patterns of the newly synthesized novel oxide obtained by Rietveld refinement has been shown in Fig. 1. The structure in packing from shown in Fig. 2. In the structure Bi(1) is bonded with Mg(15), Bi(2) bonded with O(13), Bi(2)-Bi(12), Bi(2)-Bi(12), Bi(II)–O(4), Bi(1)–O(9), Bi(2)–O(9) each forming closed type structure. The bonding between different constituent atoms has been discussed in more details in table 2.

In conclusion, the structure of $BiCa_{0.5}Mg0.5\ O_{2.5}$ has been solved by the *ab initio* approach using powder X-ray diffraction data. Bi_2O_3.CaO.MgO was found to crystalline in orthorhombic system with space group PNMA, which displays an unusual spiral chain structure along the c-axis and packing form on three-dimensional axis.

AFM investigation of $BiCa_{0.5}Mg_{0.5}O_{2.5}$ compound

Topography of $BiCa_{0.5}Mg_{0.5}O_{2.5}$ was carried out by AFM technique. It was prepared by the hydrothermal air oxidation crystallization method on a large scale (5.6×5.6 µm) is shown ion Fig. 3a, which gives the morphology of titled compound powder in a large area. The image was golden scale – encoded. That is darker regions are deeper than lighter ones and same brightness corresponding to the lights ones is not homogeneous and some powder aggregated lightly. Further information can be obtained from fig. 3b (200×200 nm), which shows the size and microstructure of $BiO_{2.5}Ca_{0.5}MgO$ aggregates. The size of the aggregates is neither the range of 2.23 nm and the shapes of the aggregates are irregular [11-12].

A typical image of sample powders, which are prepared by supercritical fluid drying, is shown in Fig. 3b (1.2×1.2 µm image). Some cone like and special particles can be seen individually in the image; the diameters of the particles is roughly 200 nm ~200 nm. It should be noted here that in imaging, rotation of the scan direction and changes of the scan frequency did not affect the structure of $BiO_{2.5}$ $Ca_{0.5}Mg_{0.5}$ particles, ruling out the possibility that scanning influenced the shapes of these particles or caused some imaging artifact. Moreover, we also found clusters of $BiO_{2.5}$ $Ca_{0.5}Mg_{0.5}$ in figure 3b. The three-dimensional figure can be seen in Fig. 3c [13, 19].The histogram (volume, area, perimeter vs. Z(nm)) of the desired compound $BiO_{2.5}$ $Ca_{0.5}Mg_{0.5}$ has been discussed in fig. 3d.

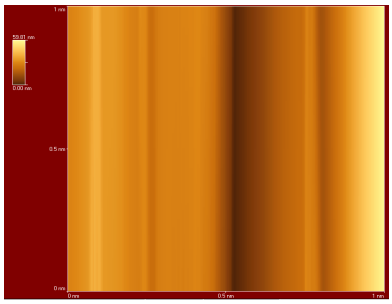

Fig.3. 1 ×1 nm AFM picture showing a rather uniform step bunching (not typical)

SEM

The SEM observation as shown in figure 4 reveals that the products consist of a large quantity of oxide with typical lengths in the wide range. The magnification SEM (500) images further verified the uniform in width and thickness.

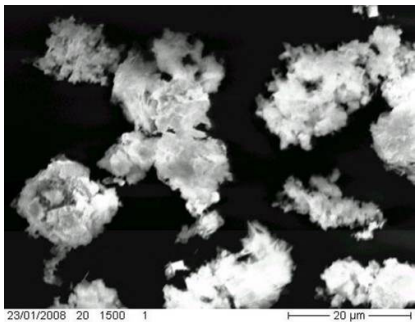

Fig 4.SEM micrograph of $BiCa_{0.5}Mg_{0.5}$ $O_{2.5}$.

Temperature dependence of the *dc* conductivity

The temperature dependence of the dc electrical conductivity of metal oxide was analyzed by complex independence method at different frequencies and in a temperature range from 20 to 110 ^{0}C in inert atmosphere.

It is observed that increase the temperature decrease the conductivity of investigated oxide due to Bi—O bond protrudes into the higher thermal parameter of O suggests a possible mode of ionic conductivity in this structure. The energy of activation was calculated by fitting the curve for the following equation

$$\sigma\ dc = \sigma_0 \exp[-\Delta E/k\ T]$$

where σ_0 is constant,K is the Boltzman constant and ΔE is the dc conduction activation energy. Value of ΔE was calculated from the slopes of the obtained straight lines indicating one conduction mechanism in the whole studied range of temperature. The value of ΔE is 0.356 eV.

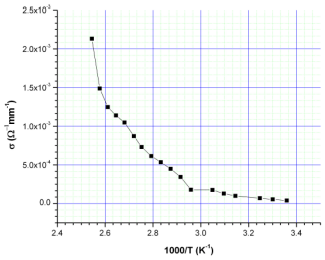

Fig. 5. The D.C. Conductivity versus temperature.

Conclusion

In conclusion, the structure of Bi2O3 MgO. CaO has been solved by the ab initio approach the using powder X-ray diffraction data.

The structure depicts, for the first time, features which are not common to the Aurivillus family of compounds.

The usual arrangements of BiO_4 units forming $(Bi_2O_2)^{2+}$ sheets in two dimensional in the Aurivillus families is restricted to a one dimensional chins in $Bi_2Ca0.5\ Mg0.5\ O2.5$.

The dc and ac conductivity are studied for the oxide compositions.

The ac conductivity of the studied compositions seems likely to be both frequency and temperature dependent.

The values of the frequency exponent s and its temperature dependence confirm the applicability of the investigated composition [20-22].

References

1. L. Y. Yong-Qiang, Ma, G.-C. Wang, J.-S. Li , G.-H. Du and J.-J. Hu Synthesis, characterization and antitumor activity of arylbismuth triphenylgermylpropionates and crystal structure of (4-$BrC_6H_4)_3Bi(O_2CCH_2CH_2GePh_3)_2and(4BrC_6H_4)_3Bi[O_2CCH(CH_3$ $CH_2GePh]_2$ *J. Organo metallic Chemistry,* 679*,* 2, 173-176, (2003) .

2. C. Guguta, H. Meekes and R. de Gelder Crystal Structure of Aspartame from Powder Diffraction Data. Crystal Growth & Design, 6, 12 ,2686-2692, (2006).

3. Swastic Mondal, Monika Mukharjee, Koushik Dhara, Souman Ghosh, Jagnyswar Rathna, Pradyot Banerjee and Alok K. Mukharjee,Supramolecular Architecture in an Oxovanadium(V)-Schiff Base complex:Synthesis,ab initio Structure Determination from X-ray Powder Diffraction, DNA Binding and Cleavage activity Crystal Growth & Design, ACSWeb 07l21l 2007, Online available.

4. Kvichiro Fukuda, Miyuki, Hisammura, Tomoyuki Iwata, Nobayuki Tera, Kimiyasu Sato, Synthesis, crystal structure and thermoelectric properties of a new carbide $Zr_2[Al_{3.56}Si_{0.44}]C_5$ J of Solid. State Chemistry , 180, 1809-1815,(2007).

5. Kinnari Parekh, Ramesh V. Upadhyay Lyubov Belova,ternary Monodispersed $Mn_{0.5}Zn_{0.5}Fe_2O_4$ ferrite nanoparticles:preparation and magnetic characterization, Nanotechnology, 17, 5910-5975, (2006).

6. Larson, A.C. Von Dreete, R.B. Los Atamos Lab, Rep. 1987, LA-UR 86, 748 (GSAS).

7. Shirley, R. The Crystfie System for Automatic Powder Indexing – 2000.

8. Digamber G. Porob and T.N. Guru Row,A Novel Oxide Ion conductor in a Doped Bi_2O_3-V_2O_5 System:Ab Initio Sturucture of New Polymorph of $NaBi_3V_2O_{10}$ via Powder x-ray diffraction, Chem. Mater,12,3658-3661.(2000),

9. Hiroshi Mizoguchi, A.P. Ramirez, L.N. Zakharov, A.W. Sleight and M.A. Subramanian,$Bi_{2/3}Ce_{1/3}Rh_2O_5$: A new mixed-valent Rh oxide with hitherto unknownstructure,J.Solid state chemistry,181,1,56-60,(2008).

10. S.L. Samal, W. Green, S.E. Lofland, K.V. Ramanujachary, D. Das and A.K. Ganguli ,Study on the solid solution of $YMn_{1-x}Fe_xO_3$: Structural, magneticanddielectricproperties,J.Solid State Chemistry, 181,1,61-66(2008)

11. N.Henry,M.Evain,P.deniard,S.Jobic,O.Mentre and F.Abraham, [Bi6O4.5(OH)3.5]2(NO3)11a new anhydrous bismuth basic nitrate Synthesis and structure determination from twinned crystals,J.solid state chemistry,2003,176,127-136

12. V. Kahlenberg, B. Marter, J.C. Munoz Aceveo, J. Patarin,Ab initio crystal structure determination of $Na_2Si_3O_7$ from conventional powder diffraction date , Solid State Sciences, 4, 1285-1292, (2002).

13. G. Herro, B.M.Epelbaum, R.Weingarther, M. Bickermann, P. Masri, A. Winnacker, Structure and dynamics of Langmuir-Blodgette tristearin films:AFM and theoretical analysis,J.Crystal Growth, 270, 113-120,(2004),.

14. Kateryna V. Terebilenko, Igor V. Zatovsky, Nikolay S. Slobodyanik, Konstantin V. Domasevitch, Denis V. Pushkin, Vyacheslav N. Baumer and Valentina S. Sudavtsova Phase relations in the system K_2MoO_4–KPO_3–MoO_3–Bi_2O_3:J.solid State chemistry,180,12,3351-3359,(2007)

15. Zhang Zhen He, Yutaka Veda, Mitsuru Itoh, Synthesis,structu and magnetic properties of new vanadate $PbCo_2V_2O_8$,J.Solid State chemistry,180, 1770-1774. (2007),

Kusz ,K. Trzebiatowski, R.J .Barezynski, Ionic conductivity of bismuth silicate and bismuth germinate glasses Solid State Ionic, 159,293-299. (2003).

16. Molak,M.Paluch,S.Pawlus,Z.Ujma,M.Pawelczyk and I.Gruszka,Properties of (Bi1/9NA2/3)(Mn1/3Nb2/3)O3 analysed within dielectric permittivity,conductivity,electri modulus and derivative techniques approach, Phase Transitions, 79,6,447-460, (2006).

17. Xiang Ying Chen, Zhong Jie Zhang and Soon W. Lee. Selective solution-phase synthesis of BiOCl, $BiVO_4$ and δ-Bi_2O_3 nanocrystals in the reaction systemof$BiCl_3$–NH_4VO_3–NaOH,J.Solid State Chemistry181,1,166-174,(200)

18. Masatake Takahshi,Yuji Noguchi,Masaru Miyayama, Estimation of ionic and hole conductivity in bismuthnitrate polycrystals at high temperatures, Solid State Ionics, 172,325-329,(2004).

19. M.A.Afifi,M.M.-Nahass,A.E.Bekheet and I.T.ZedanDc and electrical conductivity of bulk CdSexTe1-x, PHYSICA B, 400,248-251,(2007).

20. N.Kumada,N.Takahashi and N.Kinomura Preparation and Crystal Structure of a New $LiBiO_3$ J.Solid State Chemistry 1996,126,121-126.

21. Yuan Chunbo,Yang Xiaomim, Fu Degang LuZuhong and Liu Juzheng Atomic Force Microscopic Chacterization of Ultrafine Fe_3O_4,J.Solid State Chemistry,1996,121,492-494.

22.Yuan Chunbo,Yang Xiaomim, Fu Degang LuZuhong and Liu Juzheng Atomic Force Microscopic Chacterization of Ultrafine Fe_3O_4,J.Solid State Chemistry,1996,121,492-494.

Table 1Crystallographic Data of $BiCa_{0.5}Mg_{0.5}O_{2.5}$

Formula	$BiCa_{0.5}Mg_{0.5}O_{2.5}$
FW	281.17
Crystal System	Orthorhombic
Crystal Colour	White
Space Group	PNMA
Temperature : K	298
Cell parameters	
a(Å)	23.104910
b(Å)	12.618820
c(Å)	3.033075
α(deg)	90°
β(deg)	90°
γ(deg)	90°
Volume (A^3)	884.31
Av. Eps	0.0000673
Z	2
Density	1.869 g/cm^3
Limitting indices	$0 \le h \le 11$ $1 \le k \le 6$ $0 \le 1 \le 1$
Reflection collected	1884
R indices (all data)	0.022
R_1	0.0511
wR_p	0.0159
R_p	0.01271
wR_p	0.01035
M(11)	10
F(11)	5
Particle size	2.23 nm
F(000)	3063
Fc	3158

Table2 Bond angles and bond lengths

BOND ANGLES			Bond length		
S.N.	Atoms	Actual			
			S.N.	Atoms	actual
1	O(7)-Ca(5) 2.3800				
2	Mg(6)-Ca(5)	5.6080	1	O(7)-Ca(5)	2.3800
3	O(3)-Bi(2) 2.6085		2	Mg(6)-Ca(5)	5.6080
4	O(3)-Bi(1) 2.1000		3	O(3)-Bi(2)	2.6085
5	Bi(11)-O(17)	2.1000	4	O(3)-Bi(1)	2.1000
6	O(15)-Ca(13)	2.3800	5	Bi(11)-O(17)	2.1000
7	Mg(14)-Ca(13) 3.1000		6	O(15)-Ca(13)	2.3800
8	Mg(14)-O(12)	2.5378	7	Mg(14)-Ca(13)	3.1000
9	Ca(13)-O(12)	1.5098	8	Mg(14)-O(12)	2.5378
10	Bi(11)-O(16)	2.1000	9	Ca(13)-O(12)	1.5098
11	O(16)-Bi(10)	5.0009	10	Bi(11)-O(16)	2.1000
12	Mg(14)-Bi(10) 2.8200		11	O(16)-Bi(10)	5.0009
13	O(12)-Bi(10)	2.1000	12	Mg(14)-Bi(10)	2.8200
14	Bi(11)-Bi(10)	2.9200	13	O(12)-Bi(10)	2.1000
15	O(15)-O(9)	2.3800	14	Bi(11)-Bi(10)	2.9200
16	Ca(13)-O(9)	2.3800	15	O(15)-O(9) 2.3800	1.4280
17	Bi(11)-O(8)	5.0902	16	Ca(13)-O(9)	2.3800
18	Mg(6)-Bi(2)	2.8200	17	Bi(11)-O(8)	5.0902
19	Mg(14)-O(4)	1.5787	18	Mg(6)-Bi(2)	2.8200
20	Bi(10)-O(4)	2.1000	19	Mg(14)-O(4)	1.5787
21	Bi(11)-Bi(2)	2.9200	20	Bi(10)-O(4)	2.1000
22	O(8)-Bi(2) 2.6085		21	Bi(11)-Bi(2)	2.9200
23	Ca(5)-O(3)2.3800		22	O(8)-Bi(2) 2.6085	
24	Bi(11)-O(18)	1.7314	23	Ca(5)-O(3)2.3800	
25	O(8)-Bi(1) 2.1000		24	Bi(11)-O(18)	1.7314
26	Mg(6)-O(18)	2.0000	25	O(8)-Bi(1) 2.1000	
27	Bi(2)-Bi(1)	2.9200	26	Mg(6)-O(18)	2.0000
28	Bi(11)-O(16)-Bi(10)	5.9018	27	Bi(2)-Bi(1)	2.9200
29	Ca(13)-O(15)-O(9)	60.0000			
30	O(4)-Mg(14)-Bi(10)47.3313				
31	O(4)-Mg(14)-O(12)89.1934				
32	O(4)-Mg(14)-Ca(13)04.0000				
33	Bi(10)-Mg(14)-O(12)45.7767				
34	Bi(10)-Mg(14)-Ca(13)0.5000				
35	O(12)-Mg(14)-Ca(13)8.9286				
36	Mg(14)-Ca(13)-O(15)8.9227				
37	Mg(14)-Ca(13)-O(12)4.3999				
38	Mg(14)-Ca(13)-O(9)09.5000				
39	O(15)-Ca(13)-O(12)109.5000				
40	O(15)-Ca(13)-O(9)60.0000				

41	O(12)-Ca(13)-O(9)109.5000	
42	Bi(10)-O(12)-Mg(14)4.2233	
43	Bi(10)-O(12)-Ca(13)42.5912	
54	Mg(14)-O(12)-(13)6.6715	
55	O(17)-Bi(11)-O(18)106.6785	
56	O(17)-Bi(11)-Bi(2)158.7787	
57	O(17)-Bi(11)-O(8)162.3174	
58	O(17)-Bi(11)-Bi(10)107.6480	
59	O(17)-Bi(11)-O(16)82.3262	
60	O(18)-Bi(11)-Bi(2)92.4270	
61	O(18)-Bi(11)-O(8)86.8702	
62	O(18)-Bi(11)-Bi(10)42.8362	
63	O(18)-Bi(11)-O(16)137.0709	
64	Bi(2)-Bi(11)-O(8)21.6363	
65	Bi(2)-Bi(11)-Bi(10)80.0000	
66	Bi(2)-Bi(11)-O(16)90.0000	
67	O(8)-Bi(11)-Bi(10)90.0000	
68	O(8)-Bi(11)-O(16)80.0000	
69	Bi(10)-Bi(11)-O(16)169.8574	
70	Bi(11)-Bi(10)-O(12)120.0000	
71	Bi(11)-Bi(10)Mg(14)119.9988	
72	Bi(11)-Bi(10)-O(16) 4.2408	
73	Bi(11)-Bi(10)-O(4)119.9988	
74	O(12)-Bi(10)-Mg(14)60.0000	
75	O(12)-Bi(10)-O(16)117.2394	
76	O(12)-Bi(10)-O(4)90.0000	
77	Mg(14)-Bi(10)-O(16)16.0099	
78	Mg(14)-Bi(10)-O(4)33.5573	
79	O(16)-Bi(10)-O(4)117.7625	
80	O(15)-O(9)-Ca(13)60.0000	
81	Bi(1)-O(8)-Bi(2)75.7975	
82	Bi(1)-O(8)-Bi(11)51.6403	
83	Bi(2)-O(8)-Bi(11)24.3771	
84	O(7)-Ca(5)-Mg(6)163.4406	
85	O(7)-Ca(5)-O(3)163.4406	
86	Mg(6)-Ca(5)-O(3)33.1189	
87	Bi(1)-O(3)-Bi(2)75.7975	
88	Bi(1)-O(3)-Ca(5)104.0000	
89	Bi(2)-O(3)-Ca(5)90.0000	
90	Bi(2)-Mg(6)-Ca(5)31.6209	
91	Bi(2)-Mg(6)-O(18)90.0000	
92	Ca(5)-Mg(6)-O(18)109.5000	
93	Mg(14)-O(4)-Bi(10)99.1114	
94	Bi(11)-O(18)-Mg(6)20.2368	
95	Bi(1)-Bi(2)-O(8)44.2025	
96	Bi(1)-Bi(2)-Bi(11)90.0000	

Table3.Fraction coordinate.

Atomic parameters

Atom	Ox.	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å^2]
Bi		8d	1	0	0.05920	0.19990	0.45150	
O		8d	1	0	-0.30410	-0.11130	0.27600	
Bi		8d	1		-0.03790	-0.09450	0.52700	0.1267
O		8d	1	0	0.60230	-2.18500	1.40950	0.1267
Ca		8d	1		0.06700	0.03670	-0.38990	
O		8d	1		0.10100	-0.05700	0.24400	0.0063
Mg		8d	1	0	0.13330	9.60360	1.37280	
O		4c	.m.	0	-0.11(5)	0.1(3)	-0.8(6)	0.0(7)
O		4a	-1		0	0	0	0.0063