Synthesis, Crystal Structure and Characterization of the Barium Zinc Tellurate Disilicate: Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$

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Abstract. The new barium zinc(II) tellurate disilicate Ba$_3$Zn$_6$[TeO$_6$]-[Si$_2$O$_7$]$_2$ was synthesized by the high temperature solid state reaction of BaCO$_3$, ZnO, and SiO$_2$ with TeO$_3$•H$_2$O in a molar ratio of 3:6:4:1 in an evacuated silica tube at 820 °C. Its structure was established by single-crystal X-ray diffraction. Ba$_3$Zn$_6$[TeO$_6$]-[Si$_2$O$_7$]$_2$ crystallizes in the monoclinic system, space group *C2/m* (no. 12), with cell parameters of a = 15.975(5), b = 11.505(4), c = 5.142(2) Å, β = 107.437(5)°, V = 901.7(5) Å^3, and Z = 2. The structure of Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$ is composed of two types of zinc oxide polyhedra ([ZnO$_4$] tetrahedra and [ZnO$_6$] octahedra), [TeO$_6$] octahedra, disilicate group [Si$_2$O$_7$], [BaO$_6$] and [BaO$_7$] polyhedra. It can be described as a three-dimensional anionic network of {Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$}$^{6-}$, which is built from one-dimensional chains of [Zn$_6$TeO$_{18}$]$^{18-}$ anion interconnected by disilicate [Si$_2$O$_7$]$^{6-}$ groups with the barium cations located at the six-membered apertures of the above-mentioned anionic network.

Keywords: Barium; Zinc; Tellurates; Silicates; Crystal structure; Solid state reaction

1 Introduction

During the past two decades, metal selenites and tellurites have been of research interest to scientists in chemistry and materials [1]. The asymmetric coordination polyhedron adopted by Se^{IV} or Te^{IV} atoms may result in non-centrosymmetric structures with consequent interesting physical properties, such as non-linear optical second harmonic generation (SHG) [2−5]. Furthermore, "lone-pair" cations such as Se^{IV} and Te^{IV}, when mixed with a transition metal in the presence of halogenide anions, can be regarded as "chemical scissors" [6−9]. So far, the zinc tellurites reported include CuZn[TeO$_3$]Cl$_2$ [10], Zn$_2$[TeO$_3$]Cl$_2$ [11], Zn$_2$[Te$_3$O$_8$] [12, 13], Na$_2$Zn$_2$[TeO$_3$]$_3$[H$_2$O]$_{2.97}$ [14], NaHZn$_2$[TeO$_3$]$_3$[H$_2$O]$_{2.67}$ [15], Na$_2$Zn$_2$[TeO$_3$]$_3$ [15], Mn$_{0.56}$Ca$_{0.30}$Zn$_{0.12}$[Te$_2$O$_5$] [16] and Zn[TeO$_3$] [17]. The Te^{IV} cations may be oxidized to Te^{VI} under hydrothermal conditions or solid state reactions at high temperature, hence these systems also afforded a number of zinc tellurates, such as PbZn$_4$[SiO$_4$][TeO$_6$] [18], Cu$_3$Zn$_3$[TeO$_6$]$_2$ [19], Cu$_5$Zn$_4$[TeO$_6$]$_3$ [19], Ca$_3$Zn$_3$[TeO$_6$]$_2$ [20, 21], and Ca$_{1.5}$Zn$_{1.5}$[TeO$_6$] [21]. Our exploration of new compounds in BaO-ZnO-TeO$_2$ system led to the discovery of a new barium zinc tellurate disilicate: Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$. Herein we report on its synthesis and crystal structure.

Experimental Section

2.1 General

All of the chemicals except TeO$_3$•H$_2$O were analytically pure from commercial sources and used without further purification. BaCO$_3$, ZnO, and SiO$_2$ were purchased from Shanghai Reagent Factory. TeO$_2$ (99+%) was purchased from ACROS ORGANICS, Te(OH)$_6$ (99+%) was purchased from Fluka Chemika. TeO$_3$•H$_2$O was prepared according to a literature method by heating Te(OH)$_6$ at 200 °C overnight [22]. Its IR spectrum and that of the product were recorded on a Magna 750 FT−IR spectrometer photometer as a KBr pellet in the 4000−400 cm^{-1}. Microprobe elemental analysis was performed on a field emission scanning electron microscope (FESEM, JSM6700F) equipped with an energy dispersive X-ray spectroscope (EDS, Oxford INCA). X-ray powder diffraction (XRD) patterns (Cu Kα) were collected on a XPERT-MPD $\theta−2\theta$ diffractometer. Optical diffuse reflectance spectrum was measured with a PE Lambda 900 UV-vis spectrophotometer at room temperature. The instrument was equipped with an integrating sphere and controlled by a personal computer. The samples were ground into fine powder and pressed onto a thin glass slide holder. A BaSO$_4$ plate was used as a standard (100 % reflectance). The absorption spectra were calculated from reflectance spectra using the *Kubelka-Munk* function: α/S = $(1−R)^2/2R$ [23], where α is the absorption coefficient, S is the scattering coefficient, which is practically wavelength independent when the particle size is larger than $5\,\mu$m, and R is the reflectance. Thermogravimetric analyses (TGA) were carried out with a NETZSCH STA 449C unit at a heating rate of 10 °C/min under an oxygen atmosphere.

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2.2 Synthesis

The title compound was initially obtained by the high temperature solid state reaction of $BaCO_3$ (157.9 mg, 0.8 mmol), ZnO (130.2 mg, 1.6 mmol), and TeO_2 (191.5 mg, 1.2 mmol) in our attempt to synthesize a new quaternary phase of barium zinc tellurium(IV) oxide. The reaction mixture was thoroughly ground and pressed into a pellet, which was put into a silica tube, evacuated and sealed. This tube was heated to 760 °C for 7 days and then cooled to 350 °C at 5 °C/h before switching off the furnace. Colourless prism-shaped crystals of $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ were surprisingly obtained in very low yield (<5 %). The incorporated SiO_2 was obviously abstracted from the silica tube and oxidation to TeO_3 must have taken place. The Te^{IV} was probably oxidized to Te^{VI} by trace of O_2. After the structure analysis, a pure powder sample of $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ was prepared quantitatively by reacting a mixture of $BaCO_3 : ZnO : TeO_3 \cdot H_2O : SiO_2$ in a molar ratio of $3 : 6 : 1 : 4$ at 820 °C for 7 days in a sealed silica tube. The measured XRD powder pattern matches well with the one simulated from single crystal structure data. The measured molar ratio of $Ba : Zn : Si : Te$ by microprobe elemental analysis is $2.9 : 5.8 : 4.2 : 1.0$, which is in good agreement with the one determined from single crystal X-ray structure analysis. IR data (KBr, cm^{-1}): 1011 (vs), 947 (vs), 904 (s), 859 (vs), 747 (s), 659 (vs), 576 (s), 547 (s), 487 (s), 472 (s), 423 (w), 416 (w).

2.3 X-ray crystallography

The data collection for $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ was performed on Rigaku Mercury CCD (Mo-Kα radiation, graphite monochromator) at 293(2) K. The data were corrected for Lorentz factors, polarization, air absorption, and absorption due to variations in the path length through the detector faceplate. Absorption correction based on a multi-scan technique was also applied [24]. The space group was determined to be $C2/m$ (no. 12) based on systematic absences, E-value statistics, and subsequent successful refinements of the crystal structure. The structure itself was solved by direct methods (SHELXTL) and refined by least-squares methods with

Table 1 Summary of crystal data and structure refinement for $Ba_3Zn_6[TeO_6][Si_2O_7]_2$

Empirical formula	$Ba_3Zn_6TeSi_4O_{20}$
Formula weight / g·mol^{-1}	1364.20
Crystal size /mm^3	$0.36 \times 0.10 \times 0.08$
Crystal system	monoclinic
Space group	$C2/m$ (no. 12)
a /Å	15.975(5)
b /Å	11.505(4)
c /Å	5.142(2)
β /deg	107.437(5)
V /Å^3	901.7(5)
Z	2
D_c /g·cm^{-3}	5.025
μ /mm^{-1}	16.228
F(000)	1232
T /K	298(2)
λ(Mo-Kα) /Å	0.71073
Reflections collected	3529
Unique reflections	1083
Number of refined parameters	87
Goodness-of-fit (on F^2)	1.094
R_1, wR_2 (I > 2σ(I))$^{a)}$	0.0229, 0.0484
R_1, wR_2 (all data)$^{a)}$	0.0278, 0.0504
$\Delta\rho_{min}$ and $\Delta\rho_{max}$ /e Å^{-3}	0.894 and −0.895

$^{a)}$ $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, $wR_2 = \{\Sigma w[(F_o)^2 - (F_c)^2]^2 / \Sigma w[(F_o)^2]^2\}^{1/2}$.

Table 2 Atomic coordinates and U_{eq} ($10^3 \times$ Å^2) for $Ba_3Zn_6[TeO_6][Si_2O_7]_2$

Atom	site symmetry	x/a	y/b	z/c	$U_{eq}$$^{a)}$
Ba(1)	4i	0.2873(1)	1/2	0.2512(1)	12(1)
Ba(2)	2b	1/2	0	0	16(1)
Zn(1)	4h	1/2	0.3433(1)	1/2	9(1)
Zn(2)	8j	0.6434(1)	0.2801(1)	0.1731(1)	9(1)
Si	8j	0.6498(1)	0.1311(1)	0.6583(2)	6(1)
Te	2a	1/2	1/2	0	5(1)
O(1)	8j	0.7499(2)	0.1345(3)	0.6598(7)	14(1)
O(2)	8j	0.5901(2)	0.2254(3)	0.4489(7)	14(1)
O(3)	8j	0.6420(2)	0.1367(3)	0.9654(6)	12(1)
O(4)	4i	0.4301(3)	1/2	0.6350(8)	13(1)
O(5)	8j	0.5703(2)	0.3828(3)	0.8938(6)	11(1)
O(6)	4i	0.6097(3)	0	0.5362(9)	9(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3 Selected bond lengths (in Å) and angles (in °) for Ba_3Zn_6-$[TeO_6][Si_2O_7]_2$

Ba(1)−O(4)	2.530(5)	Ba(1)−O(1)#1	2.814(4)
Ba(1)−O(1)#2	2.814(4)	Ba(1)−O(3)#3	2.824(4)
Ba(1)−O(3)#4	2.824(4)	Ba(1)−O(5)#5	2.927(4)
Ba(1)−O(5)#6	2.927(4)	Ba(1)−O(1)#3	3.303(4)
Ba(1)−O(1)#4	3.303(4)	Ba(2)−O(6)#7	2.789(5)
Ba(2)−O(6)#1	2.789(5)	Ba(2)−O(3)#8	2.809(4)
Ba(2)−O(3)#4	2.809(4)	Ba(2)−O(3)#3	2.809(4)
Ba(2)−O(3)#9	2.809(4)		
Zn(1)−O(5)#10	2.050(3)	Zn(1)−O(2)#11	2.052(4)
Zn(1)−O(2)#12	2.052(4)	Zn(1)−O(4)#5	2.333(3)
Zn(1)−O(4)#13	2.333(3)	Zn(1)−O(5)	2.050(3)
Zn(2)−O(5)	1.954(3)	Zn(2)−O(3)#12	1.961(3)
Zn(2)−O(2)	1.964(3)	Zn(2)−O(1)#15	1.931(3)
Si(1)−O(1)	1.598(4)	Si(1)−O(6)	1.684(2)
Si(1)−O(2)	1.622(4)	Si(1)−O(3)	1.622(4)
Te(1)−O(4)#19	1.874(4)	Te(1)−O(5)#16	1.935(3)
Te(1)−O(4)	1.874(4)	Te(1)−O(5)#20	1.935(3)
Te(1)−O(5)#21	1.935(3)	Te(1)−O(5)#22	1.935(3)
O(5)−Zn(1)−O(5)#10	154.4(2)	O(5)−Zn(1)−O(2)#11	102.6(1)
O(5)#10−Zn(1)−O(2)#11	94.3(1)	O(5)−Zn(1)−O(2)#11	94.3(1)
O(5)#10−Zn(1)−O(2)#12	102.6(1)	O(2)#11−Zn(1)−O(2)#12	97.2(2)
O(5)−Zn(1)−O(4)#5	87.4(1)	O(5)#10−Zn(1)−O(4)#5	72.8(1)
O(2)#11−Zn(1)−O(4)#5	165.0(2)	O(2)#12−Zn(1)−O(4)#5	93.2(1)
O(5)−Zn(1)−O(4)#13	72.8(1)	O(5)#10−Zn(1)−O(4)#13	87.4(1)
O(2)#11−Zn(1)−O(4)#13	93.2(1)	O(2)#12−Zn(1)−O(4)#13	165.0(2)
O(4)#5−Zn(1)−O(4)#13	78.8(2)	O(1)#15−Zn(2)−O(5)	105.8(2)
O(1)#15−Zn(2)−O(3)#12	122.3(2)	O(5)−Zn(2)−O(3)#12	101.7(1)
O(1)#15−Zn(2)−O(2)	110.9(2)	O(5)−Zn(2)−O(2)	115.6(1)
O(3)#12−Zn(2)−O(2)	100.8(2)		
O(1)−Si−O(2)	112.0(2)	O(1)−Si−O(6)	107.0(2)
O(1)−Si−O(3)	111.3(2)	O(2)−Si−O(3)	114.7(2)
O(2)−Si−O(6)	105.6(2)	O(3)−Si−O(6)	105.5(2)
O(4)#19−Te−O(4)	180.0	O(4)−Te−O(5)#16	93.5(1)
O(4)#19−Te−O(5)#20	86.5(1)	O(4)−Te−O(5)#20	93.5(1)
O(4)#19−Te−O(5)#21	93.5(1)	O(4)−Te−O(5)#21	86.5(1)
O(4)#19−Te−O(5)#22	93.5(1)	O(4)−Te−O(5)#22	86.5(1)
O(5)#21−Te−O(5)#22	88.4(2)	O(4)#19−Te−O(5)#16	86.5(1)
O(5)#20−Te−O(5)#16	88.4(2)	O(5)#21−Te−O(5)#16	180.0
O(5)#20−Te−O(5)#22	180.0(2)	O(5)#22−Te−O(5)#16	91.6(2)
O(5)#20−Te−O(5)#21	91.6(2)		
Si−O(1)−Zn(2)#15	139.8(2)	Si−O(2)−Zn(2)	113.5(2)
Si−O(2)−Zn(1)#25	130.8(2)	Si(1)−O(3)−Zn(2)#25	124.9(2)
Zn(2)−O(2)−Zn(1)#25	110.7(2)	Zn(1)#5−O(4)−Zn(1)#21	101.2(2)
Zn(2)−O(5)−Zn(1)	128.4(2)	Si−O(6)−Si#22	127.1(3)
Te−O(4)−Zn(1)#5	96.0(2)	Te−O(4)−Zn(1)#21	96.0(2)
Te#13−O(5)−Zn(2)	118.9(2)	Te#13−O(5)−Zn(1)	103.9(2)

Symmetry code: #1: x−1/2, y−1/2, z−1; #2: x−1/2, −y+1/2, z−1; #3: x−1/2, −y+1/2, z−2; #4: x−1/2, y−1/2, z−2; #5: −x+1, −y+1, −z+1; #6: −x+1, y−1, −z+1; #7: −x+1/2, −y+1/2, −z+1; #8: −x+1/2, −y+1/2, −z+2; #9: −x+1/2, y−1/2, −z+2; #10: −x+1, y, −z+1; #11: −x+1, y, −z+2; #12: x, y−1, z; #13: x, y+1, z; #14: x, y+1, z−1; #15: −x+3/2, −y+3/2, −z+3; #16: −x+1, −y+1, −z+2; #17: x+1/2, y+1/2, z+1; #18: x+1/2, y+1/2, z+2; #19: −x+1, −y, −z+2; #20: −x+1, y−1, −z+2; #21: x, y−1, z; #22: x, −y+1, z; #23: x, y−1, z+1; #24: −x+1, −y, −z+1; #25: x, y, z+1.

atomic coordinates and anisotropic thermal displacement parameters [24] (see Table 2). The crystallographic data collection and refinement parameters are summarized in Table 1. Selected bond lengths and angles are listed in Table 3. Further details of the crystal structure investigations can be obtained from the Fachinformationszentrum Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany (fax: (49) 7247-808-666; e-mail: crysdata@fiz-karlsruhe.de), on quoting the depository number CSD−416231.

3 Results and Discussion

Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$ represents the first barium zinc tellurate disilicate. Its crystal structure features a three-dimensional anionic network of {Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$}$^{6-}$ built up from one-dimensional chains of [Zn$_6$TeO$_{18}$]$^{18-}$ interconnected by [Si$_2$O$_7$]$^{6-}$ anions (Figure 1). Alternatively it can

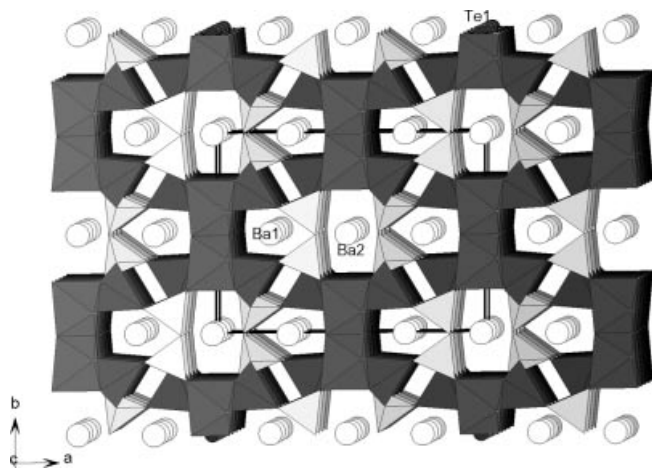**Figure 1** View of the crystal structure of Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$ down the *c*-axis. The [ZnO$_4$] tetrahedra and [ZnO$_6$] octahedra are shaded in dark gray, the [SiO$_4$] tetrahedra in light gray. Barium and tellurium atoms are represented by open and hatched circles, respectively.

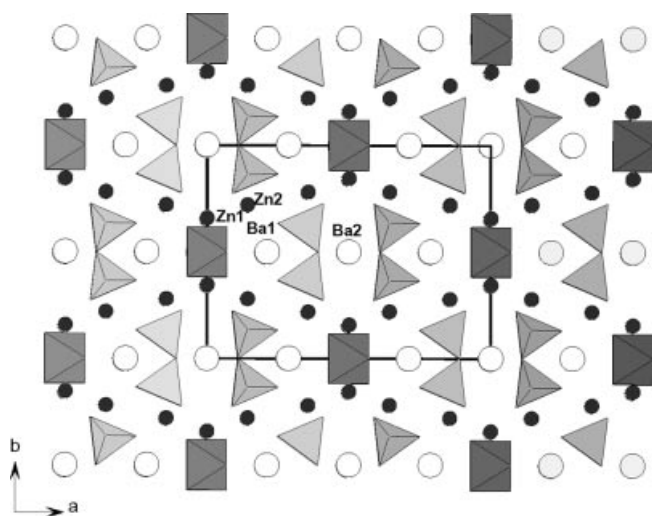**Figure 2** Packing of cations (Ba^{2+} and Zn^{2+}) and anions ([TeO$_6$]$^{6-}$ and [Si$_2$O$_7$]$^{6-}$) in Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$. The [TeO$_6$] octahedra and the [SiO$_4$] tetrahedra are shaded in medium and light gray, respectively. Ba^{2+} and Zn^{2+} cations are represented by open and hatched circles, respectively.

be described as the cations (Ba^{2+} and Zn^{2+}) surrounded by two types of anions ([TeO$_6$]$^{6-}$ and [Si$_2$O$_7$]$^{6-}$) (Figure 2). There are two unique zinc atoms, one tellurium and one silicon atom present in the asymmetric unit of Ba$_3$Zn$_6$-[TeO$_6$][Si$_2$O$_7$]$_2$. Zn(1) is octahedrally coordinated by six oxygen atoms. The axial Zn−O distances of 2.333(3) Å are significantly longer than the Zn−O bonds of the square plane (2.052(4) − 2.050(3) Å, (see Table 3). Zn(2) is tetrahedrally surrounded by four oxygen atoms with Zn−O distances ranging from 1.931(4) to 1.964(3) Å. These Zn−O distances are comparable to those reported for other zinc tellurates [18−21]. It is uncommon that an inorganic compound contains both [ZnO$_4$] tetrahedra and [ZnO$_6$] octahedra simultaneously. The tellurium(VI) cation is octahedrally coordinated by six oxygen atoms with Te−O distances in the range of 1.874(4) − 1.935(3) Å, which are comparable to those reported for other zinc tellurates [18−19]. Results of the bond valence calculations indicate that tellurium is really in the +6 oxidation state [25], for the calculated total bond valence sums up to 6.057. The Si^{IV} atom is tetrahedrally coordinated by four oxygen atoms with Si−O distances ranging from 1.598(4) to 1.684(2) Å, which are comparable to those reported in PbZn$_4$[SiO$_4$][TeO$_6$] and other zinc silicates [18, 26−28].

Two [Zn(1)O$_6$] octahedra are interconnected via common edge-sharing (O(4)...O(4)) into a dimeric unit with a Zn(1)−O(4)−Zn(1) bond angle of 101.2(2)°. Each pair of such dimeric units is bridged by four [Zn(2)O$_4$] tetrahedra via shared corners (O(2) and O(5)), resulting in a [Zn$_3$O$_9$]$^{12-}$ zinc-oxide chain along *c*-axis. The Zn(2)−O(2)−Zn(1) and Zn(2)−O(5)−Zn(1) bond angles are 110.7(2) and 128.4(2)°, respectively (Table 3). Such a connectivity also results in the formation of a number of octahedral voids within the chain, and these are occupied by tellurium(VI) cations (Figure 3). The Zn−O−Te bond angles range from 95.9(2) to 118.9(2)°.

Two neighbouring [SiO$_4$] tetrahedra are interconnected via a common corner (O(6)) to form a [Si$_2$O$_7$]$^{6-}$ dimer anion. The bond angle of the Si−O(6)−Si bridge is 127.1(3)°. Similar [Si$_2$O$_7$]$^{6-}$ anions have been reported in the lanthanoid(III) sulfide disilicates [29]. The zinc tel-
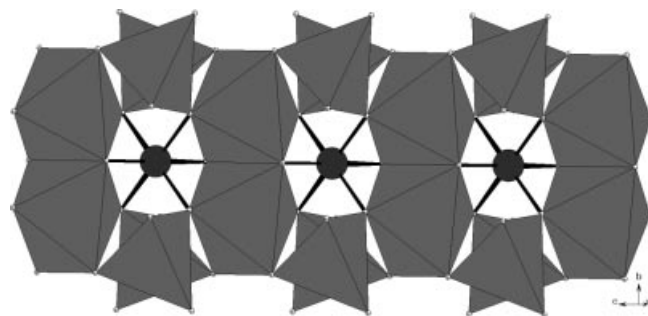

Figure 3 A one-dimensional chain of [Zn$_6$TeO$_{18}$]$^{18-}$ along *c* axis built by [ZnO$_4$] tetrahedra, [ZnO$_6$] octahedra and [TeO$_6$] octahedra in Ba$_3$Zn$_6$[TeO$_6$][Si$_2$O$_7$]$_2$. The [ZnO$_4$] tetrahedra and [ZnO$_6$] octahedra are shaded in gray. Tellurium atoms are drawn as hatched circles.
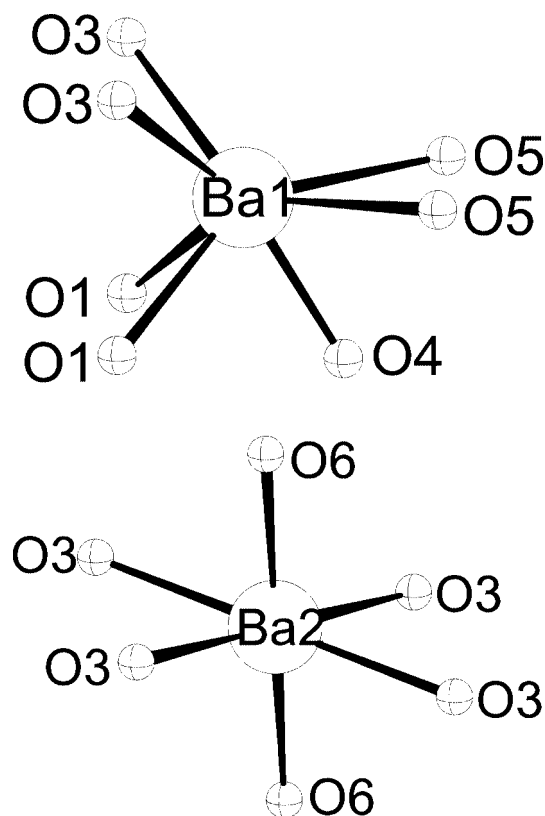
Figure 4 Coordination geometries around the barium(II) cations.

Figure 5 TGA diagram for $Ba_3Zn_6[TeO_6][Si_2O_7]_2$.
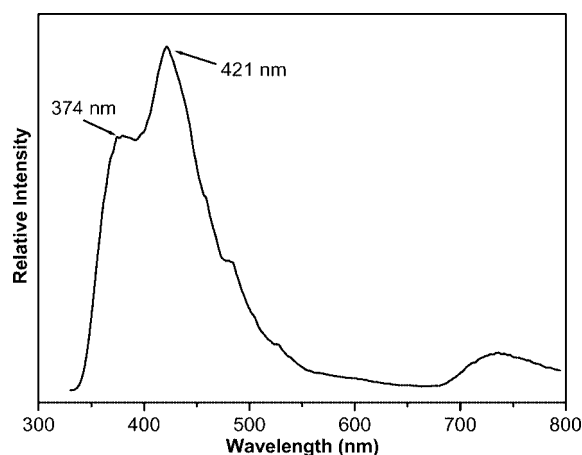
Figure 6 Emission spectrum of $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ under excitation at $\lambda_{ex} = 300$ nm.

lurium(VI) oxide chains are bridged by these $[Si_2O_7]^{6-}$ anions by corner-sharing into an open three-dimensional framework (Figure 1). The Si−O−Zn bond angles range from 113.5(2) to 139.8(2)°. Three types of apertures are thereby formed, based on four-membered rings Zn_2Si_2, as well as six-membered rings Zn_2Si_4 and Zn_4Si_2, respectively (Figure 1). Alternatively, the anionic network can also be described as though the Zn^{II} cations would be bridged by $[TeO_6]^{6-}$ and $[Si_2O_7]^{6-}$ anions.

The barium(II) cations are located at the above-mentioned six-membered apertures of the anionic network. Ba(1) resides within the six-membered apertures composed of two $[ZnO_6]$ octahedra, two $[ZnO_4]$ tetrahedra and two $[SiO_4]$ tetrahedra, whereas Ba(2) occupies the six-membered apertures built up by two $[Si_2O_7]^{6-}$ anions and two $[ZnO_6]$ octahedra. Thus Ba(1) is coordinated by seven oxygen atoms in a mono-capped trigonal prismatic geometry, whereas the coordination sphere around Ba(2) is a slightly distorted octahedron (Figure 4). The Ba−O distances are in the range of 2.530(5) − 2.927(4) Å (Table 3). It should be noted that there are also some weak Ba^{2+} - O^{2-} contacts in ranges between 3.30 and 3.80 Å which complete the extended coordination spheres of these very large cations (coordination number up to 12). Such weak Ba−O bonds include Ba(1)−O(1) (3.303(5) Å), Ba(1)−O(2) (3.793(5) Å) and Ba(1)−O(6) (3.563(5) Å) for Ba(1) cation, and Ba(2)−O(2) (3.483(5) Å) and Ba(2)−O(6) (3.356(5) Å) for Ba(2) cation.
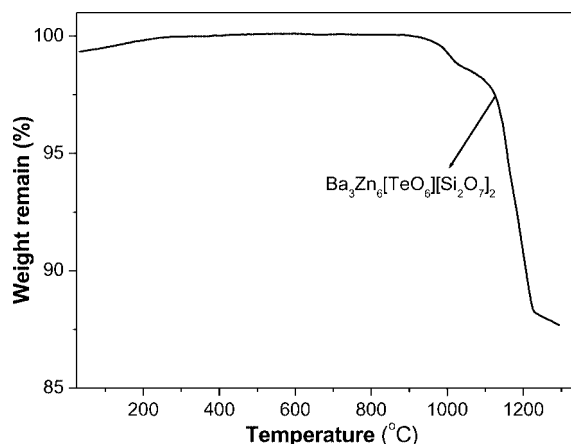
The IR spectrum of $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ exhibits absorption bands at 1011, 947, and 904 cm^{-1} which can be assigned to v(Si−O) vibrations, and those at 747, 659, 576, and 547 cm^{-1} are characteristic of v(Te−O) vibrations. Absorption peaks at 423 and 416 cm^{-1} are originating from v(Te−O−M) vibrations. All of the assignments are consistent with those previously reported [30].

Thermogravimetric analysis (TGA) under an oxygen atmosphere indicates that $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ is stable up to 950 °C, then it loses weight continuously up to 1220 °C corresponding to the release of TeO_3 (Figure 5). The total weight loss of 12.4 % at 1220 °C is close to the calculate value (12.9 %). The residual was not further characterized.

Optical diffuse reflectance spectrum of $Ba_3Zn_6[TeO_6]$-$[Si_2O_7]_2$ reveals the presence of an optical band gap of 4.4 eV. Hence the compound is an insulator.

The solid state luminescent property of $Ba_3Zn_6[TeO_6]$-$[Si_2O_7]_2$ has been also investigated at room temperature. Under excitation of 300 nm, it displays two emission bands: a strong one at 421 nm and a shoulder band at 374 nm (Figure 6). Both bands are probably originated from the LMCT absorption [31].

4 Conclusion

In conclusion, the synthesis, crystal structure, and characterization of $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ have been described. $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ features a three-dimensional anionic network of $\{Zn_6[TeO_6][Si_2O_7]_2\}^{6-}$ which is built up from one-dimensional chains of $[Zn_6TeO_{18}]^{18-}$ interconnected by $[Si_2O_7]^{6-}$ anions via corner sharing. Optical diffuse reflectance spectrum of $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ reveals that $Ba_3Zn_6[TeO_6][Si_2O_7]_2$ is an insulator. Future research efforts will be devoted to the preparation of analogous barium zinc tellurate germanates.

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