ANALYSIS OF THE CRYSTAL STRUCTURE OF THE Ba$_3$TeO$_6$ COMPOUND

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Abstract

The object of research is the crystal structure of the Ba$_3$TeO$_6$ compound. It is known from the literature that this material has photoluminescent properties and crystallizes in the tetragonal system with the space symmetry group I41/a (88) and lattice periods $a = 19.3878$ A; $b = 19.3878$ A°, $c = 34.909$ A°. At the same time, there are data on two other polymorphic modifications of this compound, which are in the PDF-2 database for 2009. Therefore, information about the crystal structure of this compound is incomplete. The existence of different spectra for a given compound mentioned in the literature may be due to different methods of synthesis of this compound. A study of the crystal structure of the compound Ba$_3$TeO$_6$ under the number 00-035-0995 in the PDF-2 database for 2009 is proposed.

The study used the 2009 PDF-2 database. As well as the HighScorePlus 3.0 program (Netherlands), which makes it possible to refine the microstructural parameters of a structural model using the Rietveld method.

The diffraction spectrum for the study was generated using the HighScorePlus 3.0 program and the 2009 pdf-2 database connected to it in UDF format.

As a result, it was found that this diffraction spectrum of the studied compound can correspond to the following structural model: orthorhombic system with lattice periods $a = 4.2910$ A; $b = 4.4062$ A; $c = 4.3459$ A. The space symmetry group Pnnn(48) is possible.

Analyzing the results obtained, it should be recognized that the studied structure of the compound crystallizes in its own structural type. At the same time, the crystal structures of the polymorphic modifications of this compound are similar.

The study of the crystal structure of the compound contributes to a better understanding of its physical properties, in particular, photoluminescence.

Keywords: X-ray diffraction analysis, Bragg-Bertrand survey geometry, Rietveld method, crystal structure, Ba$_3$TeO$_6$ composition.

1. Introduction

The Ba$_3$TeO$_6$ compound was obtained in the form of a polycrystalline powder [1]. It has photoluminescent properties [2]. In [1], diffraction patterns were also obtained by the powder method with the Bragg-Bertrand survey geometry on copper X-rays and indexed in the orthorhombic crystal system. At the same time, information on the crystal structure of the compound is partially presented in the literature. Therefore, the study of the crystal structure of this compound is topical.

The object of research is the crystal structure of Ba$_3$TeO$_6$.

It follows from the literature sources that there are two diffraction spectra of the indicated compound obtained using X-ray powder diffraction (Bragg-Bertrand method) of different quality, given in [3], for which the crystal structure is unknown. The crystal structure of the studied compound was also synthesized and proposed [4]. Therefore, this compound is characterized by polymorphism. The crystal structure of the polymorphic modification of the Ba$_3$TeO$_6$ compound, number 00-035-0995 in the PDF-2 database for 2009 [3], has not been studied.

The aim of research is to propose a structural model of the diffraction spectrum of the Ba$_3$TeO$_6$ compound under the number 00-035-0995 in the PDF-2 database for 2009 [3].

To achieve this aim, it is necessary to solve the following objectives:

1. Index the diffraction spectrum of compound number 1 (**Table 1**) using the module of the program HighScorePlus 3.0 [5] TREOR.

2. Determine the lattice periods and crystal system.

3. Choose the space symmetry group for the given spectrum of the compound.

4. Propose a structural model for the given spectrum of the compound.

5. Refine the microstructural parameters for the selected model using the Rietveld method [6].

2. Materials and methods of research

Alkali metal tellurate was prepared from TeO_2 99.9 % (LAB) (Merck) and $BaCO_3$ taken in stoichiometric ratio. The mixture was heated in air at 925 K for 24 hours and then at 1500 K for 60 hours. Barium carbonate was obtained from the corresponding nitrate with the participation of $(NH_4)_2CO_3$ [1]. The diffraction spectra of the compound are presented in the ICDD PDF-2 database for 2009 [3]. Data on the diffraction spectra of the compound in the database [3] are given in **Table 1**.

Table 1

Information about the Ba_3TeO_6 crystal structure

No.	Compound	Crystal system, ПГС	Lattice periods, A°	Card number in the pdf-2 database	Quality of the diffraction spectrum
1	Ba_3TeO_6	orthorhombic, I	$a = 8.8080$ $b = 8.6890$ $c = 8.5760$	00-035-0995	High spectrum quality
2	Ba_3TeO_6	orthorhombic, Pmmm	$a = 8.8080$ $b = 8.6890$ $c = 8.5760$	00-049-1845	Low spectrum quality

This tellurate is formed as a by-product during the synthesis of $Ba_3Co_2TeO_9$ and is defined as phase 2 in Table 1 (00-049-1845, PDF-2) according to [7]. Also, according to [7], it is a decomposition product of the $Ba_3Co_2TeO_9$ compound.

Oxidation of TeO_2 and $BaCO_3$ according to [8] yields the compound under study, which belongs to the structural type $(NH_4)_3FeF_6$.

According to [9], during the Ba_2ZnTeO_6 synthesis at a temperature of 900 °C, Ba_3TeO_6 is formed as an impurity. The presence of this phase was established by X-ray phase analysis.

The crystal structure of the Ba_3TeO_6 compound was studied in most detail in [4]. Barium tellurate was synthesized at a temperature of 1373K in air with the oxidation of TeO_2 in a $BaBr_2$ melt.

The resulting single crystals crystallize in the tetragonal system with the space symmetry group I41/a (88) and lattice periods $a = 19.3878$ A°; $b = 19.3878$ A° $c = 34.909$ A° and microstructural parameters given in [4]. The CIF file is also contained in the electronic database COD (ID 8104519) [11].

However, in [3], the diffraction spectra of the compound were obtained by the powder method with the Bragg-Bertrand survey geometry on X-ray copper filtered radiation, the structures of which are unknown.

The diffraction spectrum for the study was generated using the HighScorePlus 3.0 program [5] and the connected pdf-2 database for 2009 [3] in UDF format.

Obtaining initial data for the study of the crystal structure of the compound was used exclusively by data taken from the PDF-2 database for 2009 [3]. This database contains experimental diffractograms of different «quality» taken by the powder method with the Bragg-Bertrand survey geometry. Each sample is given an identification number.

The analysis of the proposed structural model of this spectrum was also carried out using the HighScorePlus 3.0 program using the Rietveld method.

3. Results and discussion

The diffraction spectrum of the compound is indexed in orthorhombic crystal system with lattice periods $a = 4.2910$ A°; $b = 4.4062$ A°; $c = 4.3459$ A°. The space symmetry group Pnnn(48) is possible. The refined microstructural characteristics for the studied range of the compound are given in **Table 2**. The values of interplanar distances and intensity, which are given in [3] and calculated using this model, are given in **Table 3**.

Discrepancy factor – $R = 6.3591$ %.

Table 4 shows the interatomic distances of the proposed structural model for the Ba_3TeO_6 compound numbered 00-037-0738 in the pdf-2 database for 2009.

Table 2

Microstructural parameters of Ba_3TeO_6

Atom	Correct point system	x	y	z	Position fill rate	U_{iso}^a
Ba	4h	0.097912	0.250000	0.750000	0.150	10.0(3)
Te	2a	0.2500000	0.250000	0.250000	0.100	10.0(3)
O	4j	0.750000	0.937316	0.2500000	0.300	3.0(1)

Table 3

The values of interplanar distances and intensities given in [3] and calculated using this model

d_{cal} (A°)	d_{obs} (A°)	I_{cal}	I_{obs}	H	K	L
3.09141	3.09160	64.58	63.47	0	1	1
3.07147	3.07187	100.00	100.00	1	1	0
3.05081	3.05217	32.28	60.38	1	0	1
2.50796	2.50895	0.00	2.10	1	1	1
2.20177	2.20200	13.22	14.18	0	2	0
2.17166	2.17200	29.79	18.27	0	0	2
2.14427	2.14499	1.17	12.21	2	0	0
1.78576	1.78597	0.07	0.93	1	2	1
1.77359	1.77360	14.54	17.50	1	1	2
1.76229	1.76208	3.26	10.23	2	1	1
1.54645	1.54610	2.70	2.01	0	2	2
1.53647	1.53591	0.25	5.16	2	2	0
1.52613	1.52579	0.42	4.12	2	0	2
1.45483	–	0.00	–	1	2	2
1.44858	–	0.00	–	2	2	1
1.44206	–	0.00	–	2	1	2
1.39095	1.39074	0.09	1.05	0	3	1
1.38912	–	0.24	–	1	3	0
1.37570	1.37571	0.76	3.01	0	1	3
1.37207	1.37213	0.55	2.11	1	0	3
1.36001	1.35962	0.20	2.04	3	1	0
1.35821	1.35780	0.58	3.28	3	0	1
1.32316	–	0.00	–	1	3	1
1.31001	–	0.00	–	1	1	3
1.29793	–	0.00	–	3	1	1

Table 4

Interatomic distances of the Ba_3TeO_6 compound

Atom1	Atom2	Distance, A°
Te	– Ba	2.269
Te	– O	2.324
Te	– O	2.550
Te	– Ba	2.661
Ba	– O	1.052
Ba	– Ba	1.305
Ba	– Te	2.269
Ba	– Te	2.661
Ba	– O	2.975
Ba	– Ba	2.986
Ba	– Ba	3.206
O	– Ba	1.052
O	– O	1.651
O	–Te	2.324
O	– Te	2.550
O	– O	2.755
O	– Ba	2.975

Fig. 1 shows diffraction pattern generated and calculated according to the structural model for the Ba_3TeO_6 compound. **Fig. 2** shows an image of the proposed model of the crystal structure of the compound under study.
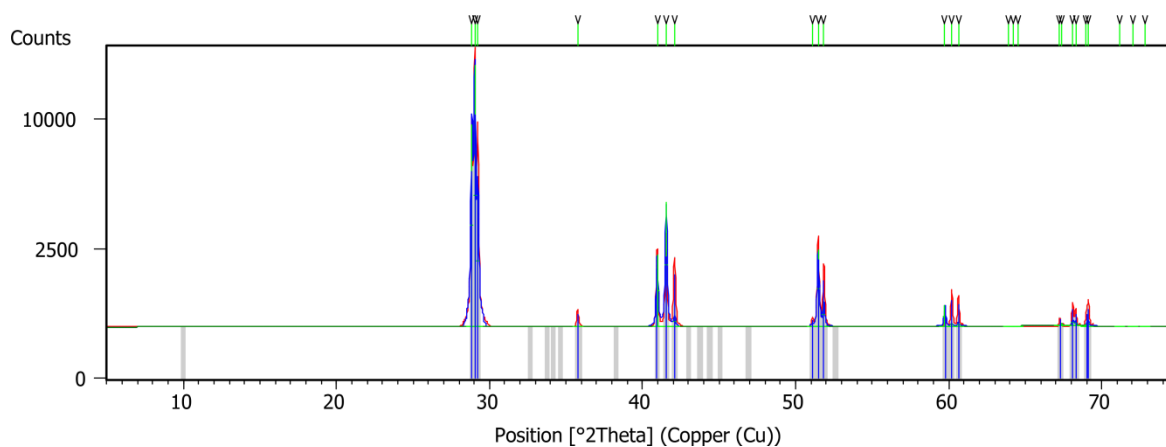

Fig. 1. The resulting diffraction pattern of the Ba_3TeO_6 compound was generated and calculated using the structural model
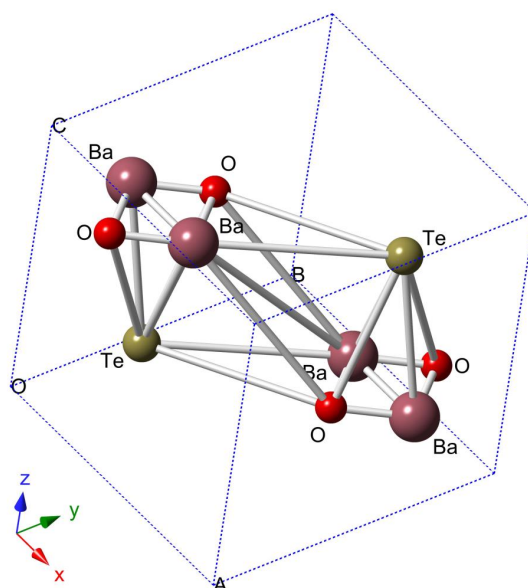

Fig. 2. Crystal structure of the Ba_3TeO_6 compound for the studied diffraction spectrum

It follows from the results obtained that barium atoms form bonds with oxygen and tellurium atoms and with themselves. Oxygen atoms are bonded to tellurium and barium atoms, and tellurium to oxygen and barium. Tellurium is located at the top of the pyramid formed by the atoms of barium and oxygen, the compound under study (**Fig. 2**).

Also it is noted that, according to [3] and [4], this compound is characterized by polymorphism. It is found in [4] that the compound crystallizes in the tetragonal crystal system, and in [3] the diffraction spectrum of the compound is given, according to the results of processing given in [3], as well as in this work, refers to the orthorhombic crystal system. Microstructural parameters are proposed and presented in this work.

Despite the fact that the crystal structures of polymorphic modifications of the studied compound belong to different crystal systems, their structures are similar. Thus, according to [4], TeO_6 and BaO_6 atoms form octahedral polyhedra.

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For the studied structure of the Ba_3TeO_6 compound, barium, oxygen, and tellurium atoms form pyramids at the vertices of which there are tellurium atoms (**Fig. 2**).

The correct systems of points of the studied structure are partially filled (**Table 2**).

There is information about the presence of several diffraction spectra of this compound (orthorhombic and tetragonal crystal system), and various methods for the formation of the studied compound. It is possible that the method of obtaining this compound affects its type of crystal structure.

Also, partial filling of the correct systems of points in the structure under study may indicate that the stoichiometric composition of the compound may be slightly changed.

4. Conclusions

Using the program module [5] TREOR, indexing of the X-ray diffraction pattern of the Ba_3TeO_6 compound under the number 00-037-0738 in the pdf-2 database for 2009 was carried out.

The diffraction spectrum of the compound is indexed in orthorhombic crystal system with lattice periods $a = 4.290$ A°; $b = 4.401$ A°; $c = 4.342$ A°. The space symmetry group Pnnn(48) is possible.

The diffraction spectrum of the compound Ba_3TeO_6 under the number 00-037-0738 in the pdf-2 database for 2009 was studied using the HighScorePlus 3.0 program [5] by the Rietveld method. A structural model has been proposed: space symmetry group Pnnn (48), lattice periods $a = 4.2910$ A°; $b = 4.4062$ A°; $c = 4.3459$ A°. Discrepancy factor $- R = 6.3591$ %. Microstructural characteristics are given in **Table 2**.

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