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REFINEMENT OF MICROSTRUCTURAL PARAMETERS OF THE CRYSTAL STRUCTURE OF COMPOUND BA_2MOO_5

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Barium molybdates have a wide range of applications: in nuclear power, photoluminescent devices, solid-state lasers, photocatalysts, and gas sensing. They are used in microwave and thermoelectric devices. Ba_2MoO_5 belongs to this group of compounds. Several methods for its production are known from the literature. Ba_2MoO_5 is obtained by reactions: $BaMoO_4+BaCO_3 \rightarrow Ba_2MoO_5+CO_2$, $BaMoO_4+Ba_3MoO_6 \rightarrow 2Ba_2MoO_5$. This chemical can also be obtained from the reaction of $BaMoO_4$ with Mo and BaO_2. Ba_2MoO_5 and Mo, $BaMoO_4$ were formed, which did not react. According to the state diagram of $BaO\text{-}MoO_3$, it borders on $Ba_3Mo_7O_{24}$ and $BaMoO_4$. It has a melting point of 1280^0 C in the eutectic and 1370 °C in the melt. The presence of Ba_2MoO_5 was determined by X-ray phase analysis using the database of powder diffractograms with the Brag-Brentano geometry, PDF-2. The spectrum of the compound is available in the card 025-0011. The synthesis of the compound whose diffraction spectrum is reported in card 025-0011, PDF-2 database (ICDD) for 2009 was the result of the reaction of $BaCO_3$ and MoO_3, taken in a molar ratio of 2:1, placed in a gold crucible and heated to 900 °C and kept in air for 4 days. From the analysis of the literature, it follows that Ba_2MoO_5 crystallizes in orthorhombic syngony, has the Pnma symmetry group, lattice periods a = 7.4097A°, b = 5.7603A°, c = 11.3906A° and belongs to the $K_2VO_2F_3$ structure type. Using the above information on the crystal structure of the studied compound, the microstructural parameters were refined using the spectrum published in card 025-0011 of the PDF-2 (ICDD) database for 2009. The values of the lattice periods were refined: a=7.408471A°, b=5.734523A°, c=11.469570A°, spatial symmetry group Pnma. Microstructural parameters: Ba(1) 4c x/a=0.178307; y/b=0.250000; z/c=0.416387; position filling factor s.o.f.=1; Ba(2) 4c x/a=0.482515; y/b=0.250000; z/c=0.715824; s.o.f.=1; Mo(1) 4c x/a= 0.1585(9); y/b=0.250000; z/c= 0.0671(5); s.o.f.=1; O(1) 4a x/a= 0; y/b=0; z/c= 0; s.o.f.=1; O(2) 4c x/a=0.731075; y/b=0.250000; z/c=-0.001550; s.=1; O(3) 4c x/a=0.336331; y/b=0.250000; z/c=0.904934; s.o.f.=1; O(4) 8d x/a=0.267908; y/b=0.134197; z/c=0.053091; s.o.f.=1.

Key words: *crystal structure, Rietveld method, compound Ba_2MoO_5.*

Заводянний В. В. Уточнення мікроструктурних параметрів кристалічної структури сполуки Ba_2MoO_5

Молібдати барію мають широкий спектр застосування: в ядерній енергетиці, фотолюмінесцентних пристроях, твердотільних лазерах, фотокаталізаторах, зондуванні газу. Застосовуються в мікрохвильових та термоелектричних пристроях. До цього ряду сполук належить і Ba_2MoO_5. Із літератури відомо декілька методів її отримання. Ba_2MoO_5 отримують за реакціями: $BaMoO_4+BaCO_3 \rightarrow Ba_2MoO_5+CO_2$, $BaMoO_4+Ba_3MoO_6 \rightarrow 2Ba_2MoO_5$ Також дану хімічну речовину можна отримати в результаті реакції $BaMoO_4$ з Mo і BaO_2 Утворювалися Ba_2MoO_5 і Mo, $BaMoO_4$ які не прореагували. Відповідно до діаграми стану $BaO\text{-}MoO_3$ вона межує з $Ba_3Mo_7O_{24}$ та $BaMoO_4$. Має температуру плавлення 1280 °C за евтектикою, і 1370 °C з розплаву. Присутність Ba_2MoO_5 визначалась в результаті рентгенівського фазового аналізу за допомогою бази даних порошкових дифрактограм з геометрією зйомки Брег-Брентано, PDF-2. Спектр сполуки міститься в картці 025-0011. Синтез сполуки, дифракційний спектр якої міститься в картці 025-0011, бази даних PDF-2 (ICDD) за 2009 рік відбувався в результаті реакції BaCO3 і MoO3, взятих в молярному співвідношені 2:1, розміщених в золотому тиглі і нагрітих до 9000С та витриманих протягом 4 діб на повітрі. З аналізу літературних джерел слідує, що Ba2MoO5 кристалізується в орторомбічній сингонії, має просторову групу симетрії Pnma, періоди решітки a=7,4097A0, b=5,7603A0, c=11,3906A0 і належить до типу структури $K_2VO_2F_3$. Використовуючи зазначені відомості про кристалічну структуру досліджуваної сполуки було проведено уточнення мікроструктурних параметрів за спектром розміщеним в картці 025-0011 бази даних PDF-2 (ICDD) за 2009 рік. Уточнені значення періодів решітки: a=7,408471A0, b=5,734523A0, c=11,469570A0, просторова група симетрії Pnma.

Мікроструктурні параметри: Ba(1) 4c x/a=0,178307; y/b=0,250000; z/c=0,416387; коефіцієнт заповнення позицій s.o.f.=1; Ba(2) 4c x/a=0,482515; y/b=0,250000; z/c=0,715824; s.o.f.=1; Mo(1) 4c x/a= 0,1585(9); y/b=0,250000; z/c= 0,0671(5); s.o.f.=1; O(1) 4a x/a= 0; y/b=0; z/c= 0; s.o.f.=1; O(2) 4c x/a=0,731075; y/b=0,250000; z/c=-0,001550; s.o.f.=1; O(3) 4c x/a=0,336331; y/b=0,250000; z/c=0,904934; s.o.f.=1; O(4) 8d x/a=0,267908; y/b=0,134197; z/c=0,053091; s.o.f.=1.

Ключові слова: *кристалічна структура, метод Рітвельда, сполука* Ba_2MoO_5.

Introduction. Compounds of the Ba-Mo-O system have a wide range of properties. For example, they are used in nuclear power, photoluminescence, solid-state lasers, photocatalysts, gas sensing, microwave and thermoelectric properties [1]. The compound Ba_2MoO_5 is one of the representatives of this class. Therefore, the study of the properties and structure of this compound, in particular its crystal structure, is relevant.

The symmetry and lattice periods of this compound were determined and reported in [2]. Namely, the structure of Ba_2MoO_5 was assigned to the rhombic syngony with lattice periods *a = 7.*412 A°, *b = 5.*769 A°, *c = 11.*380 A°.

The method for obtaining this compound is reported in detail in [3]. The compound can be obtained by reactions:

$$BaMoO_4 + BaCO_3 \rightarrow Ba_2MoO_5 + CO_2$$

$$BaMoO_4 + Ba_3MoO_6 \rightarrow 2\ Ba_2MoO_5$$

The phase diagram of BaO-MoO is given in [4]$_3$ Fig. 1.

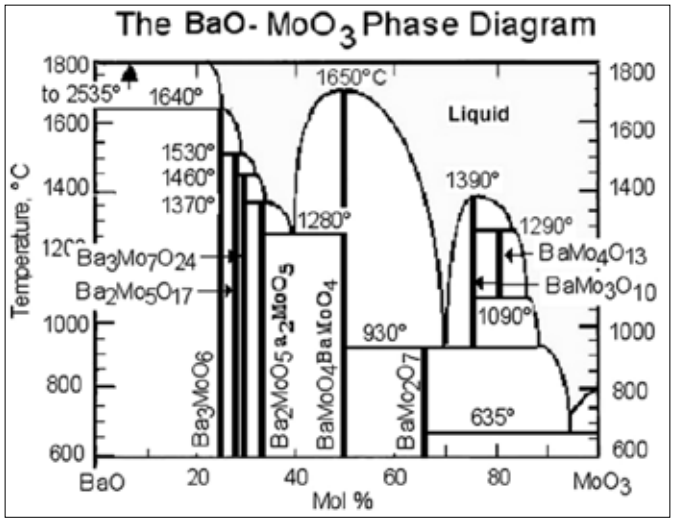

Fig. 1. Phase diagram of BaO-MoO_3

According to it, the compound has a melting point of 1280 ℃ in the eutectic and 1370 ℃ in the melt.

Also, as a result of the reaction of $BaMoO_4$ with Mo and BaO_2, Ba_2MoO_5 and Mo, $BaMoO_4$ were formed, which did not react [5].

In [6], the compound $Ba_2\ MoO_5$ card 25-0011 JCPDS was observed by X-ray phase analysis using the PDF-2 database.

The aim of this work is to clarify the microstructural parameters of the compound $Ba_2\ MoO_5$.

Research results. Information on the crystal structure of this compound can be found in [7]. The samples for the study were prepared from $BaCO_3$ and MoO_3 in a molar ratio of 2:1, heated to 900 °C in a gold crucible and kept in air for 4 days. $Ba_2 MoO_5$ crystallizes in rhombic syngony, with the *Pnam* symmetry group, Z = 4, and belongs to the structural type $K_2VO_2F_3$, and has lattice periods *a = 7*.4097(7)A°*, b = 11*.3906(8)A°*, c = 5*.7603(6) A° [7].

These data were taken as the initial ones for the structural model of the compound under study. The microstructural parameters $K_2VO_2F_3$ are given in Table 1. Spatial symmetry group *Pnma*, lattice periods *a* = 7.415(1)A°, *b* = 5.7637(6)A°, *c* = 11.391(2)A° [8].

Table 1

Microstructural parameters $K_2VO_2F_3$

Atom	Wyck.	s.o.f.	*x*	*y*	*z*
K(1)	4c	1,000000	0,190800	0,250000	0,592880
K(2)	4c	1,000000	0,477500	0,250000	0,282940
V	4c	1,000000	0,199500	0,250000	0,306000
O	8d	1,000000	0,177800	0,523300	0,389400
F(1)	4a	1,000000	0,000000	0,000000	0,000000
F(2)	4c	1,000000	0,037100	0,250000	0,805700
F(3)	4c	1,000000	0,272600	0,250000	0,091500

The diffraction spectrum of the compound was obtained from the PDF-2 database for 2009 under the number 25-0011, taken at copper filtered radiation with a wavelength of л = 1.54060A° , with the Breg-Brentano survey geometry in UDF format.

The microstructural parameters were determined by the Rietveld method using the HighScore Plus 3.0 program.

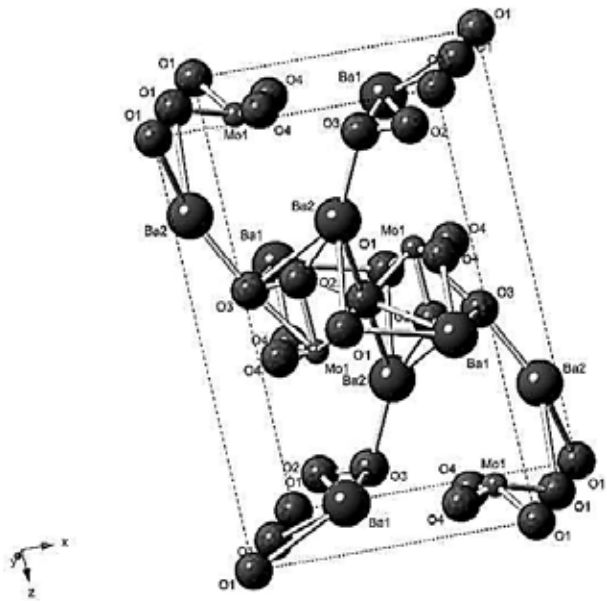

Fig. 2. Crystal structure of Ba compound$_2$ MoO_5

Microstructural parameters are shown in Table 2.

Table 2

Microstructural parameters of the structure of compound Ba_2MoO_5

Atom	Wyck.	s.o.f.	*x*	*y*	*z*
Ba1	4c	1,000000	0,178307	0,250000	0,416387
Ba2	4c	1,000000	0,482515	0,250000	0,715824
Mo1	4c	1,000000	0,1585(9)	0,250000	0,0671(5)
O1	4a	1,000000	0,000000	0,000000	0,000000
O2	4c	1,000000	0,731075	0,250000	-0,001550
O3	4c	1,000000	0,336331	0,250000	0,904934
O4	8d	1,000000	0,267908	0,134197	0,053091

The compound belongs to the orthorhombic syngonium, the spatial symmetry group is *Pnma*, the refined lattice periods are a = 7.408471A°, b = 5.734523A°, c = 11.469570A°. The discrepancy factor is R = 8.11 %.

Conclusion. The crystal structure of the compound Ba_2MoO_5 was studied by the diffraction spectrum obtained in [7] and given in the PDF-2 database for 2009 (ICDD) under the number 025-0011, taken on a copper filtered radiation with a wavelength of л = 1.54060A^0 and a Breg-Brentano survey geometry.

The structure of the compound belongs to the orthorhombic syngonium, the *Pnma* symmetry group, with lattice periods a = 7.408471A°, b = 5.734523A°, c = 11.469570A°.

Microstructural parameters are shown in Table 2. The discrepancy factor is R = 8.11 %. The compound belongs to the structural type $K_2VO_2F_3$.

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