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. \( \text{Ba}_2\text{MoO}_5 \) belongs to this group of compounds. Several methods for its production are known from the literature. \( \text{Ba}_2\text{MoO}_5 \) is obtained by reactions: 
\[
\text{BaMoO}_4 + \text{BaCO}_3 \rightarrow \text{Ba}_2\text{MoO}_5 + \text{CO}_2
\]
\[
\text{BaMoO}_4 + \text{Ba}_3\text{MoO}_6 \rightarrow 2\text{Ba}_2\text{MoO}_5
\]
This chemical can also be obtained from the reaction of \( \text{BaMoO}_3 \) with Mo and \( \text{BaO}_2 \). \( \text{Ba}_2\text{MoO}_5 \) and Mo, \( \text{BaMoO}_4 \) were formed, which did not react. According to the state diagram of \( \text{BaO}-\text{MoO}_3 \), it borders on \( \text{Ba}_3\text{Mo}_7\text{O}_{24} \) and \( \text{BaMoO}_4 \). It has a melting point of 1280°C in the eutectic and 1370°C in the melt. The presence of \( \text{Ba}_2\text{MoO}_5 \) was determined by X-ray phase analysis using the database of powder diffractograms with the Bragg-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 \( \text{BaCO}_3 \) and \( \text{MoO}_3 \), 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 \( \text{Ba}_2\text{MoO}_5 \) crystallizes in orthorhombic symmetry, lattice periods \( a = 7.4097 \text{ Å}, b = 5.7603 \text{ Å}, c = 11.3906 \text{ Å} \) and belongs to the \( \text{K}_2\text{VO}_2\text{F}_3 \) 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: \( a = 7.408471 \text{ Å}, b = 5.734523 \text{ Å}, c = 11.469570 \text{ Å} \), spatial symmetry group \( \text{Pnma} \). Microstructural parameters: \( \text{Ba}(1) 4\text{c} x/a=0.178307; y/b=0.250000; z/c=0.416387; \) \( \text{position filling factor s.o.f.=1; Ba}(2) 4\text{c} x/a=0.482515; y/b=0.250000; z/c=0.715824; s.o.f.=1; \) \( \text{Mo}(1) 4\text{c} x/a=0.1585(9); y/b=0.250000; z/c=0.0671(5); s.o.f.=1; \) \( \text{O}(1) 4\text{a} x/a=0; y/b=0; z/c=0; s.o.f.=1; \) \( \text{O}(2) 4\text{c} x/a=0.320000; y/b=0.250000; z/c=0.094594; s.o.f.=1; \) \( \text{O}(3) 8\text{d} x/a=0.267908; y/b=0.134197; z/c=0.053091; s.o.f.=1. \)
**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 \( \text{Ba}_2\text{MoO}_5 \) 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 \( \text{Ba}_2\text{MoO}_5 \) was assigned to the rhombic syngony with lattice periods \( a = 7.412 \text{ Å}, b = 5.769 \text{ Å}, c = 11.380 \text{ Å} \).

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

\[
\begin{align*}
\text{BaMoO}_4 + \text{BaCO}_3 & \rightarrow \text{Ba}_2\text{MoO}_5 + \text{CO}_2 \\
\text{BaMoO}_4 + \text{Ba}_2\text{MoO}_6 & \rightarrow 2 \text{ Ba}_2\text{MoO}_5
\end{align*}
\]

The phase diagram of \( \text{BaO-MoO}_3 \) is given in [4], Fig. 1.

![Phase diagram of \( \text{BaO-MoO}_3 \)](image)

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

Also, as a result of the reaction of \( \text{BaMoO}_4 \) with \( \text{Mo} \) and \( \text{BaO}_2 \), \( \text{Ba}_2\text{MoO}_5 \) and \( \text{Mo} \), \( \text{BaMoO}_4 \) were formed, which did not react [5].

In [6], the compound \( \text{Ba}_2 \text{MoO}_5 \) 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 \( \text{Ba}_2 \text{MoO}_5 \).
**Research results.** Information on the crystal structure of this compound can be found in [7]. The samples for the study were prepared from BaCO₃ and MoO₃ in a molar ratio of 2:1, heated to 900 °C in a gold crucible and kept in air for 4 days. Ba₂MoO₅ crystallizes in rhombic syngony, with the Pnam symmetry group, Z = 4, and belongs to the structural type K₂VO₂F₃, and has lattice periods \(a = 7.4097(7)\,\text{Å}, b = 11.3906(8)\,\text{Å}, c = 5.7603(6)\,\text{Å}^2[7].

These data were taken as the initial ones for the structural model of the compound under study. The microstructural parameters K₂VO₂F₃ are given in Table 1. Spatial symmetry group Pnma, lattice periods \(a = 7.415(1)\,\text{Å}, b = 5.7637(6)\,\text{Å}, c = 11.391(2)\,\text{Å}^2[8].

### Table 1

<table>
<thead>
<tr>
<th>Atom</th>
<th>Wyck.</th>
<th>s.o.f.</th>
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<th>(y)</th>
<th>(z)</th>
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<td>0,091500</td>
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</table>

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 \(\lambda = 1.54060\,\text{Å}\), 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.
Microstructural parameters are shown in Table 2.

### Table 2

<table>
<thead>
<tr>
<th>Atom</th>
<th>Wyck.</th>
<th>s.o.f.</th>
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<th>y</th>
<th>z</th>
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</tr>
</tbody>
</table>

The compound belongs to the orthorhombic syngonium, the spatial symmetry group is *Pnma*, the refined lattice periods are \( a = 7.408471 \text{Å}, \ b = 5.734523 \text{Å}, \ c = 11.469570 \text{Å} \). The discrepancy factor is \( R = 8.11 \% \).

**Conclusion.** The crystal structure of the compound Ba₂MoO₅ 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 \( \lambda = 1.54060 \text{Å} \) and a Breg-Brentano survey geometry.

The structure of the compound belongs to the orthorhombic syngonium, the *Pnma* symmetry group, with lattice periods \( a = 7.408471 \text{Å}, \ b = 5.734523 \text{Å}, \ c = 11.469570 \text{Å} \).

Microstructural parameters are shown in Table 2. The discrepancy factor is \( R = 8.11 \% \). The compound belongs to the structural type K₂VO₂F₃.

**BIBLIOGRAPHY:**

8. Ryan R.R., Mastin S.H., Reisfeld M. J. The crystal structure of K₂VO₂F₃, a non-linear dioxovanadium (V) group. *Acta Crystallographica Section B Structural Crystal-
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