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Article

Synthesis and Analysis of the Optical Properties of the Perovskite Material $KPBBR_3$ Studying the Characteristics and Potential for Application.

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Abstract: Perovskite materials such as $KPbBr_3$ hold a special place in modern material science and optoelectronics due to their optical and electronic properties. The relevance of studying this material can be justified by the following factors. $KPbBr_3$ possesses significant optical properties such as a wide bandgap and high fluorescence. This makes it a promising material for use in devices such as LEDs, photodetectors, and solar cells. Unlike other perovskites, $KPbBr_3$ is composed of relatively accessible and inexpensive components. This makes it attractive for mass production and commercialization, which is especially important for the development of cost-effective optoelectronic devices. Varying the ratio of starting components in the synthesis of $KPbBr_3$ allows for control over its optical properties, opening up broad possibilities for optimizing the material for specific applications.

Keywords: $KPbBr_3$, perovskite, synthesis, optical properties, absorption spectroscopy, fluorescence, IR spectroscopy.

Introduction

The development of new materials for use in solar cells and other sustainable energy devices is one of the priority tasks of modern science. $KPbBr_3$, due to its properties, has the potential to become a key component in the creation of more efficient and durable solar cells. Investigating the structure and optical properties of $KPbBr_3$ contributes to the fundamental understanding of the mechanisms underlying the behavior of perovskite materials.

The study of the perovskite material $KPbBr_3$ is highly relevant both from scientific and practical perspectives, offering promising opportunities for innovative advancements in the fields of optoelectronics and sustainable energy.

Materials and Methods

Perovskite materials, such as $KPbBr_3$, have garnered significant attention due to their unique optical properties and potential applications in the field of optoelectronics. $KPbBr_3$ is an important perovskite material with a cubic crystal structure, characterized by high light absorption and

luminescence values [1–5]. Various synthesis methods, such as the reactive melt method and solution precipitation, influence the quality and optical properties of $KPbBr_3$ [6,7]. Studies show that the optical characteristics of $KPbBr_3$, including absorption and luminescence spectra, depend on synthesis conditions and component ratios [8]. $KPbBr_3$ exhibits promising potential for use in various optoelectronic devices, such as LEDs and solar cells [9–11]. Further research is required to optimize the properties and stability of $KPbBr_3$, as well as to study its interactions with other materials [12]. $KPbBr_3$ is a promising material for use in modern optoelectronic technologies, and continued investigation may unveil new opportunities for its application. Exploring various synthesis methods for $KPbBr_3$, such as the reactive melt method and solution precipitation, is essential for producing a material with high purity, uniform structure, and controlled optical properties. This approach opens new prospects for its use in photonics and optoelectronics. Determining the key optical properties of $KPbBr_3$, including absorption and luminescence spectra, as well as their dependence on synthesis conditions and initial component ratios, is a crucial step in advancing its application potential [13-14].
Solutions of KBr and $PbBr_2$ in DMSO were prepared at concentrations sufficient for the formation of $KPbBr_3$ crystals. The experiments utilized component ratios of 1:1 (23.8 mg KBr and 37.9 mg $Pb(CH_3COO)_2 \cdot 3H_2O$) and 2:1 (59.5 mg KBr and 94.75 mg $Pb(CH_3COO)_2 \cdot 3H_2O$).
The solutions were mixed at a temperature of 75 ºC, leading to the formation of $KPbBr_3$ crystals. The solution was filtered using syringe filters. The formed crystals were observed under a UV lamp, where light scattering was detected.
Absorption spectra were recorded in the range of 200 to 800 nm. Samples obtained with different component ratios were analyzed to identify variations in their optical properties.
The samples were excited with ultraviolet light, and luminescence spectra were measured in the visible range. For comparison, samples synthesized with KBr:PbBr ratios of 1:1 and 2:1 were used (Figures 1–4).
Infrared spectra were analyzed in the high-frequency range of 3200–3600 cm^{-1} down to the low-frequency region below 500 cm^{-1} (Figures 5 and 6).

Results and Discussions

The data obtained from each synthesis and investigation were thoroughly analyzed and compared. Particular attention was given to comparing the optical properties of samples synthesized with different component ratios. The results were presented as absorption and luminescence spectra, along with images of the crystal morphology.

These methods provided a comprehensive understanding of the structure and optical properties of the perovskite material $KPbBr_3$, as well as the influence of synthesis conditions on its characteristics.

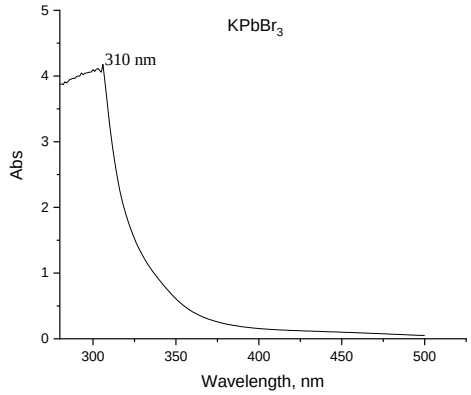

Fig. 1. Absorption spectrum of $KPbBr_3$ at a reagent ratio of 1:1.

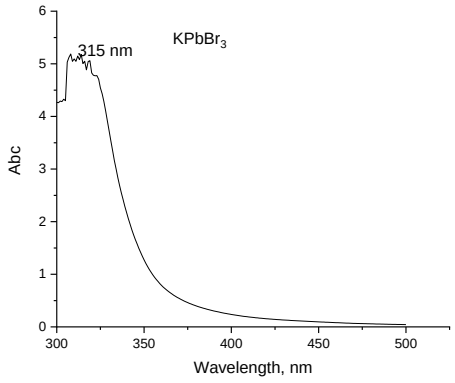

Fig. 2. Absorption spectrum of $KPbBr_3$ at a reagent ratio of 2:1.

Figure 1 presents the absorption spectrum of $KPbBr_3$ at a $KBr:PbBr_2$ ratio of 1:1. The spectrum exhibits broad absorption in the ultraviolet range with a maximum at 310 nm, corresponding to an energy gap of 3.0 eV. The spectrum for the 2:1 ratio (Figure 2) demonstrates similar characteristics; however, a slight shift towards lower absorption is observed, which may be attributed to changes in the crystal structure or morphology of the material.

In the context of perovskite materials such as $KPbBr_3$, shifts in the absorption wavelength are associated with changes in the crystal structure, the presence of defects, impurities, or variations in the material's composition. A shift towards longer wavelengths (from 310 nm to 315 nm) results from changes in synthesis conditions, indicating alterations in crystal quality and morphology.

The luminescence spectra for $KPbBr_3$ (Figures 3 and 4) revealed pronounced fluorescence with a maximum in the visible range. At a $KBr:PbBr_2$ ratio of 2:1, an increase in fluorescence intensity was observed compared to the 1:1 ratio.

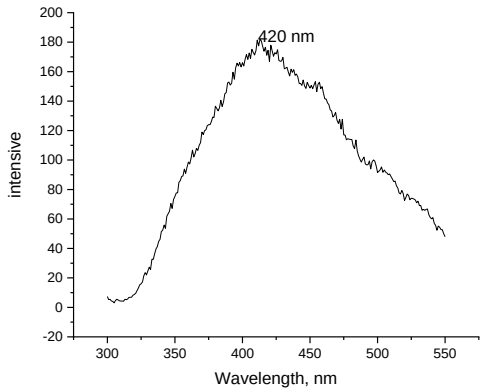

Fig. 3. Luminescence spectrum of $KPbBr_3$ at a reagent ratio of 1:1.

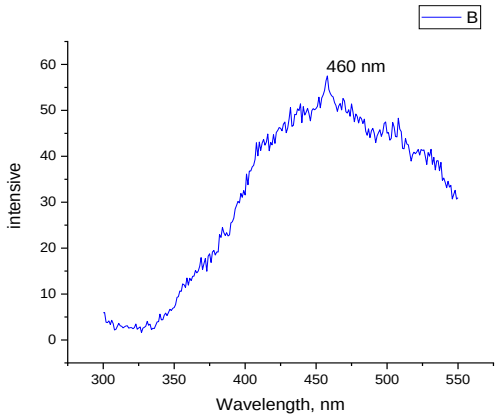

Fig. 4. Luminescence spectrum of $KPbBr_3$ at a reagent ratio of 2:1.

The increase in luminescence intensity with changes in the component ratio may be attributed to improved crystal quality, resulting in reduced carrier recombination losses.

Data analysis revealed that the KBr to $PbBr_2$ ratio significantly influences the optical properties of $KPbBr_3$. At a 2:1 ratio, a decrease in both absorption and luminescence of the material is observed, which may be associated with more efficient formation of the perovskite structure and a reduction in defects. This is because the luminescence spectrum changes depending on the concentration of luminescent centers or active molecules. High concentrations promote intermolecular interactions, leading to a red shift in the luminescence spectrum.

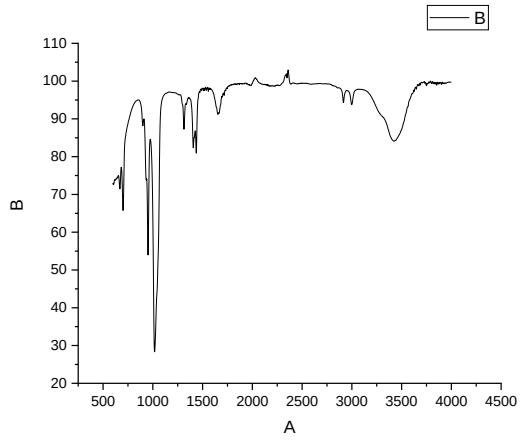

Fig. 5. Infrared spectrum of $KPbBr_3$ at a reagent ratio of 1:1.

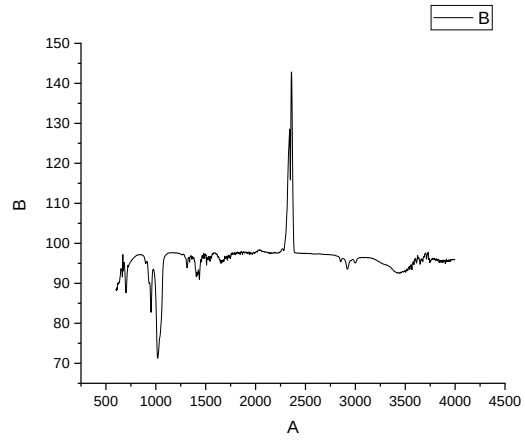

Fig. 6. Infrared spectrum of $KPbBr_3$ at a reagent ratio of 2:1.

Based on the infrared spectrum of the $KPbBr_3$ complex stabilized with oleic acid, as presented in Figure 5, the following conclusions can be drawn:

In the high-frequency region of 3200–3600 cm^{-1}, absorption associated with the stretching vibrations of O-H groups can be observed, indicating the presence of oleic acid in its free form. However, the presence of both broad and narrow bands suggests the degree of interaction between the acid and the complex. For the stretching vibrations of C-H bonds in the aliphatic chains of oleic acid, the range of 2850–2950 cm^{-1} is a typical region. The presence of intense bands in this area confirms the existence of long hydrocarbon chains. The absorption band in the 1700–1750 cm^{-1} range corresponds to the vibrations of the C=O bond in the carboxyl group of oleic acid. In the low-frequency region (<500 cm^{-1}), absorption bands corresponding to the vibrations of Pb-Br and K-Br bonds are observed, which are characteristic of heavy metals and halides. These bands are crucial for confirming the formation of the complex structure.

The analysis of the IR spectra of the $KPbBr_3$ complex stabilized with oleic acid, as shown in Figure 6, reveals absorption bands in the 2850–2950 cm^{-1} region corresponding to the stretching vibrations of C-H bonds in the aliphatic chains of oleic acid. This confirms the presence of the hydrocarbon chain characteristic of oleic acid, which acts as a stabilizer for the complex. The band in the 1700–1750 cm^{-1} region is associated with the stretching vibrations of the C=O bond in the carboxyl group of oleic acid.

The shift and change in intensity of this band indicate the interaction of the carboxyl group with the metal in the complex. This is characteristic of the coordination of the carboxyl group of oleic acid to lead in $KPbBr_3$. Bands in the low-frequency region (<700 cm^{-1}) may be associated with the stretching vibrations of Pb-Br and K-Br bonds, which are typical for lead and bromine complexes. These bands confirm the presence of these chemical bonds within the structure of the complex. In the 3000–3600 cm^{-1} region, bands related to the vibrations of O-H groups can be observed. This suggests that most of the oleic acid is in a coordinated form, interacting with the complex rather than remaining free. The IR spectrum indicates the presence of oleic acid stabilizing the $KPbBr_3$ complex and features characteristic bands that demonstrate the interaction of the acid's carboxyl group with lead ions, as well as the presence of Pb-Br and K-Br bonds.

Conclusion

1. Crystals of the perovskite material $KPbBr_3$ were successfully synthesized using the solution precipitation method. Ultraviolet-visible spectroscopy revealed that $KPbBr_3$ exhibits broad absorption in the ultraviolet range with an energy gap of 3.0 eV.
2. Fluorescence spectroscopy revealed pronounced luminescence in the material, which intensified when the KBr:$PbBr_2$ ratio was adjusted to 2:1. Altering the ratio of KBr to $PbBr_2$ during synthesis significantly affects the optical properties of the material. The 2:1 ratio results in improved absorption and luminescence, attributed to enhanced crystal structure quality and reduced defects.
3. Recommendations for further research on $KPbBr_3$ include several key directions: continuing the exploration of various synthesis methods to optimize the crystalline structure and material purity, investigating the effects of different impurities and additives on the optical properties, and experimentally studying the stability of the material under various operational conditions.
4. Efforts should focus on developing new perovskite compositions with enhanced properties, conducting scalable tests to assess the industrial feasibility of $KPbBr_3$, and studying the material's interactions with other components in complex systems. Developing quality control methods and process parameters during synthesis will enhance the reliability of final

products. Additionally, attention to patenting new technologies and materials will help protect intellectual property.

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