

Synthesis and characterization of Sr₂Be₂B₂O₇ by XRD and FTIR

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In this work pure Sr₂Be₂B₂O₇ material was prepared by solid-state reaction at 950°C in air. The stoichiometric amounts of SrO, BeO and H₃BO₃ were used as starting materials. Phase analysis of the synthesized materials was carried out using powder X-ray diffraction (XRD). They were characterized by Fourier transform infrared spectroscopy (FTIR) as well.

Keywords: strontium beryllium borate, XRD, FTIR

INTRODUCTION

Pure and doped borates have been used in many areas such as germicidal drinking water purification, non-linear optics, photocopying, phototherapy, sunlamps, laundry marking, blueprinting, instrumental dial illumination, window displays, etc. [1-8].

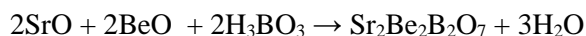
The studies that are carried on Sr₂Be₂B₂O₇ exist rarely in the literature since it is just a new compound. Investigations are usually focused on the single crystal synthesis by using different methods and NLO applications [4-8].

In this work pure Sr₂Be₂B₂O₇ material was prepared by solid-state reaction. The phase analysis of all synthesized materials was carried out using powder X-ray diffraction (XRD). Also the synthesized materials were characterized by Fourier transform infrared spectroscopy (FTIR).

EXPERIMENTAL

Pure Sr₂Be₂B₂O₇ material was prepared by a solid-state method at 950 °C in air. Stoichiometric amounts of SrO, BeO and H₃BO₃ were used as starting materials (SrO and BeO were produced by calcinations of related metal nitrates and/or carbonates). After adding suitable amount of acetone into reaction medium, the precursors were introduced into a muffle furnace and maintained at 500 °C for 2 h. The precursor powders were thoroughly mixed and then slowly heated at 950°C for 12 h in air.

Reaction:



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The XRD structural analysis of Sr₂Be₂B₂O₇ material was performed on an X-ray Phillips X'Pert Pro equipped with Cu K α (30 kV, 15 mA, λ = 1.54051 Å) radiation at room temperature. Scanning was generally performed between 10° and 90° 2 θ . Measurement was made with 0.0330° step size at 25°C.

The Fourier transform infrared spectra between 500 and 4000 cm⁻¹ were measured at room temperature with a Shimadzu 8303 FTIR spectrometer. All samples were prepared as KBr pellets.

RESULTS AND DISCUSSION

The XRD pattern of Sr₂Be₂B₂O₇ is presented in Fig. 1. It is in a full agreement with the JCPDS (82-2448).

To determine the coordination environments of both B–O and Be–O in the Sr₂Be₂B₂O₇ structure, the FTIR spectra of Sr₂Be₂B₂O₇ were measured at room temperature. As seen in Fig. 2, the strong bands observed at 614.99, 697.75 and 1241.77 cm⁻¹ should be assigned to the B–O vibrations of the triangular [BO₃] groups [1, 5, 9, 10], while the band with a peak at 890.66 cm⁻¹ should be attributed to the Be–O vibration of the tetragonal [BeO₄] group [5]. FTIR spectrum data of Sr₂Be₂B₂O₇ are listed in Table 1.

Point group of Sr₂Be₂B₂O₇ (SBBO) is D_{3h}. Geometric parameters of the synthesized borate are P6̄c2, a=b=4.683 Å, c=15.311 Å, α = β =90°, γ =120° [4, 7, 11].

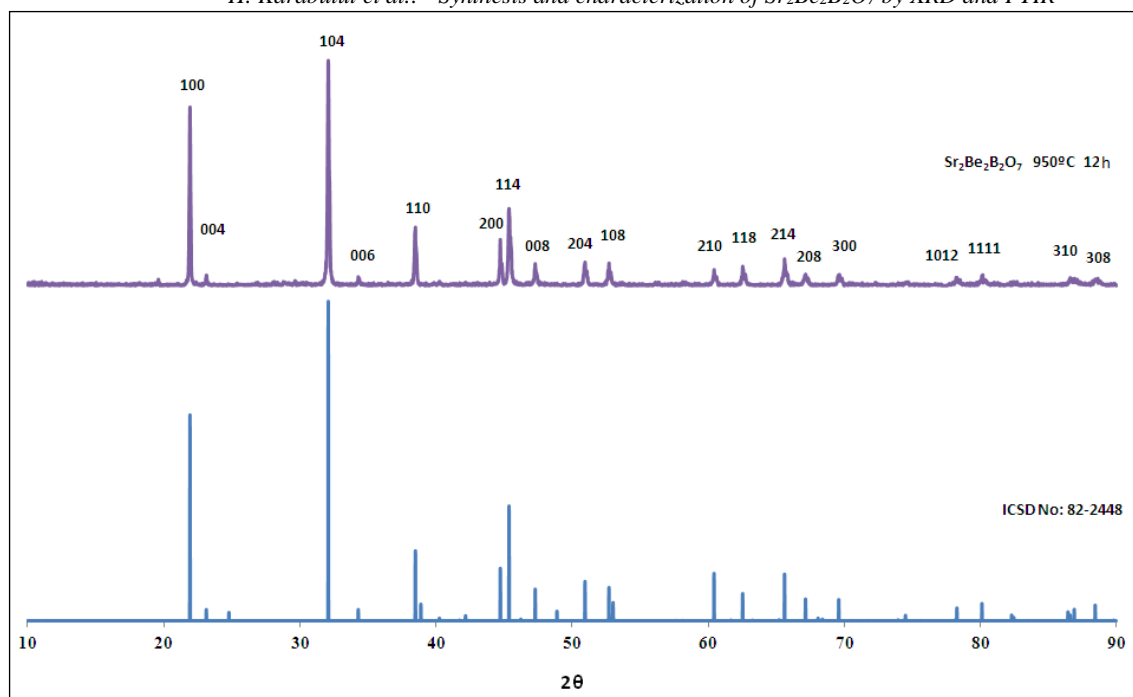


Fig. 1. XRD pattern of Sr₂Be₂B₂O₇ prepared by a solid-state synthesis

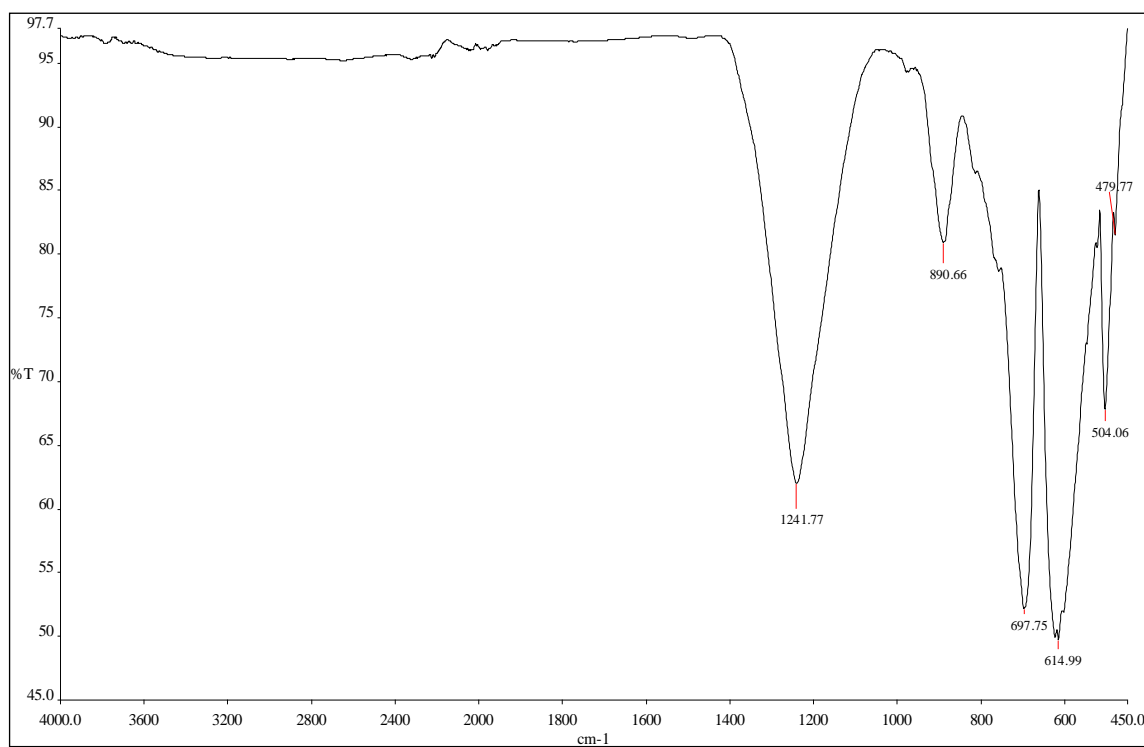


Fig. 2. Infrared spectra of Sr₂Be₂B₂O₇ prepared by a solid-state synthesis

Table 1. FTIR spectrum data of Sr₂Be₂B₂O₇

Assignments	$\nu_3(\text{BO}_3)$	$\nu_3(\text{BeO}_4)$	$\nu_2(\text{BO}_3)$	$\nu_4(\text{BO}_3)$
Frequency (cm ⁻¹)	1241.77	890.66	697.75	614.99

According to these data it can be concluded that two possible sites available for incorporating activator ions (such as Dy³⁺, Sm³⁺, Tb³⁺, Eu³⁺, Pb²⁺, etc.) in Sr₂Be₂B₂O₇ lattice are either the Sr²⁺ sites or the Be²⁺ sites. The Dy³⁺ (0.912 Å for CN = 6), Sm³⁺ (0.958 Å for CN = 6), Tb³⁺ (0.923 Å for CN = 6), and Pb²⁺ (1.19 Å for CN = 6) ions are of a much larger ionic radius, compared with that of the Be²⁺ (0.27 Å for CN = 4) ion. However, the ionic radius of Sr²⁺ (1.18 Å for CN = 6) is larger than that of the activator ions. So in the first luminescence study that was made by our research group [5], the Sr²⁺ ions in the Sr₂Be₂B₂O₇ lattice were replaced by the mentioned activator ions (Dy³⁺, Sm³⁺, Tb³⁺, Pb²⁺).

CONCLUSION

Sr₂Be₂B₂O₇ material was prepared by solid-state reaction. The phase analysis of the synthesized material was carried out using powder XRD and characterized by FTIR. The XRD pattern of the synthesized material is in agreement with the JCPDS (82-2448). Also the coordination environments of both B–O and Be–O in the Sr₂Be₂B₂O₇ structure were confirmed by FTIR measurement.

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СИНТЕЗ И ОХАРАКТЕРИЗИРАНЕ НА Sr₂Be₂B₂O₇ ПОСРЕДСТВОМ XRD И FTIR

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(Резюме)

В тази работа е получен чист материал от Sr₂Be₂B₂O₇ чрез твърдофазна реакция при 950°C във въздушна среда. Като изходни материали са използвани стехиометрични количества от SrO, BeO и H₃BO₃. С помощта на прахов рентгеноструктурен анализ (XRD) е извършен фазов анализ на синтезираните материали. Последните са охарактеризирани и чрез инфрачервена спектроскопия с Фурие-трансформация (FTIR).

Ключови думи: Стронциев берилиев борат, Рентгеноструктурен анализ, Инфрачервена спектроскопия с Фурие трансформация