

CHARACTERIZATION OF Ba(NO₃)₂, KNO₃ PURE AND DISTINCT SYSTEM

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ABSTRACT

Characterization (XRD and FTIR) measurements, being made in pellets of pure Ba(NO₃)₂, KNO₃ and in the distinct system of Ba(NO₃)₂-KNO₃ in the area of temperature ranging from lukewarm temperature to their respective systems of melting points. The conclusion points out that the conductivity in the farfetched of Ba(NO₃)₂ increased as the mole percentage of KNO₃ increased up to the mole percentage of 91 and then for mole percentage 95 conductivity falls. The activation energies are calculated for all the compositions and it is found the minimum for a 91-molepercent. Characterization by XRD patterns in the mixed system Ba(NO₃)₂ : KNO₃ reveals the presence of additional peaks and shifting in peak positions corresponding to an introduction of a new phase which indicates the solid solution formation. From FTIR also it is observed that new peaks and shift in peak positions in the mixed system of 0.19Ba(NO₃)₂ -0.81KNO₃ is observed. The system also has been investigated through DTA, DSC, and SEM. From DSC and DTA studies it is found that the melting point of disparate systems will be actually lower than that of the host systems and in this case, it is found to be at about 290^oC.

Keywords: Composite solid electrolyte, Ionic conductors, Enhancement in Conductivity, dispersoid, nanostructure, Space charge region.

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INTRODUCTION

Most of the Ionic conductors in the area of solid-state ionics are very important. The study of solid electrolytes and their uses is the study of Solid-state ionics. The materials that fall into this area include inorganic crystalline and polycrystalline solids, disparate crystals, glasses, ceramics, polymers, and composites. Mixed crystals are more favorable for enhancement of conductivity when compared to mono crystal. In order to achieve higher ionic conductivities, we have chosen the dispersion of insulating second phase particles to a mixed ionic conductor. Because some of these composite solid electrolytes exhibit high ionic conductivity and good mechanical properties and are found to be promising materials for solid-state batteries, fuel cells, electrodes etc. Solid-state ionic devices such as solid oxide fuel cells can be much more reliable and long-lasting. There exist many solids with high ionic conductivity greater than 10⁻⁴ Ω⁻¹ cm⁻¹ and they are of immense use in various technological applications.

For the ionic conductivity, transport of one or more types of ions across the material is necessary and the majority of superionic solids discovered are cation based conductors. Study of ionic transport in materials that are suitable to record higher conductivities such as mixed and composite solid electrolyte systems, is gaining importance because of the possible potential applications. The search for discovering newer materials with improved mechanical and electrical properties that come under this category continues. distinct crystals are more favorable for enhancement of conductivity when compared to monocrystal. In order to achieve higher ionic conductivities we have chosen the dispersion of insulating second phase particles to a mixed ionic conductor.

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Because some of these composite solid electrolytes exhibit high ionic conductivity and good mechanical properties and are found to be promising materials for solid-state batteries, fuel cells, electrodes etc. The work presented in this thesis covers the enhancement of conductivity in $\text{Ba}(\text{NO}_3)_2 : \text{KNO}_3$ mixed crystal

EXPERIMENTAL

X-Ray Diffractogram

XRD data collected from powder samples using an automated X-ray powder diffractometer SHIMADZU model-XRD-7000 ($K_\alpha=1.54\text{\AA}$) at room temperature for pure $\text{Ba}(\text{NO}_3)_2$, KNO_3 and their disparate systems of $_{0.62}\text{Ba}(\text{NO}_3)_2 -_{0.38}\text{KNO}_3$, $_{0.37}\text{Ba}(\text{NO}_3)_2 -_{0.63}\text{KNO}_3$, $_{0.25}\text{Ba}(\text{NO}_3)_2 -_{0.75}\text{KNO}_3$, $_{0.19}\text{Ba}(\text{NO}_3)_2 -_{0.81}\text{KNO}_3$, $_{0.05}\text{Ba}(\text{NO}_3)_2 -_{0.95}\text{KNO}_3$ mole percentages are shown in Figure 1. XRD patterns show the being of additional peaks and move in peak positions in the disparate system corresponding to a new phase which points out the configuration of solid solution¹⁻². It may also be noted that ionic radius of $\text{Ba}^{2+}(1.35\text{\AA})$ and $\text{K}^+(1.33\text{\AA})$ are nearly matched advocating the configuration of solid solution and in the present case it is confirmed that “aliovalent substitutional solid solution”. (In aliovalent solid solution, ions of different charge are substituted by other ions).

As per Vegard's law difference in lattice parameters or atomic radius of the two constituents forming solid solution should be lower than 5%³. In the present system it is found to be 3.7% with respect to ‘Ba’ and 3.85% with respect to ‘K’. The effect of solid solution configuration can be either to insert or strengthen the physical properties such as ferromagnetism, mechanical strength and conductivity etc. In solid-state ionic particularly it is the increment in ionic conductivity⁴. Figure-2a shows the schematic representation of Vegard's law in $\text{Li}_{1+x}\text{Ti}_{2-x}\text{Ga}(\text{PO}_4)_3$ system⁴. This indicates the configuration of the ideal solid solution. Figure-2b shows the solid configuration in the present disparate system $\text{Ba}(\text{NO}_3)_2 : \text{KNO}_3$. From the figure it is clear that in the present disparate system lattice parameters are varying with mole percentages.

RESULTS AND DISCUSSION

FTIR Spectroscopy

This technique is used for structural analysis. In the present study, IR spectrum of KNO_3 and $\text{Ba}(\text{NO}_3)_2$, and their disparate system of $_{0.19}\text{Ba}(\text{NO}_3)_2 -_{0.81}\text{KNO}_3$ was recorded using SHIMADZU spectrophotometer are shown in Fig.-3. The IR spectrum was recorded in the wave number range from 500-3500 cm^{-1} . In $\text{Ba}(\text{NO}_3)_2$ the sharp peaks observed at 728 cm^{-1} and 815 cm^{-1} and in KNO_3 at 826 cm^{-1} is due to the vibration of N in and out of NO_3 plane and the strongest absorption in $\text{Ba}(\text{NO}_3)_2$ at 1361 cm^{-1} and 1417 cm^{-1} and in KNO_3 at 1383 cm^{-1} due to asymmetric NO_3 stretch which confirms the presence of nitrate.

In $_{0.19}\text{Ba}(\text{NO}_3)_2 -_{0.81}\text{KNO}_3$ ⁵ also the sharp peak observed at 824 cm^{-1} is due to the vibration of N in and out of NO_3 plane and the strongest absorption at 1406 cm^{-1} is due to asymmetric NO_3 stretch which confirms the presence of nitrate. From FTIR also it is observed that new peaks and there are a shift in peak positions in the disparate system of $_{0.19}\text{Ba}(\text{NO}_3)_2 -_{0.81}\text{KNO}_3$ ⁶ as compared with pure crystals i.e., $\text{Ba}(\text{NO}_3)_2$ and KNO_3 ⁷. This supports the X-ray powder patterns in which we not only observed new peaks but also there is a shift in peak positions of disparate systems. From the XRD and spectral analysis, it is clear that the existence of additional peaks corresponds to a new phase which indicates the configuration of solid solution⁸.

CONCLUSION

The present disparate system $\text{Ba}(\text{NO}_3)_2 : \text{KNO}_3$ has been investigated through XRD, and FTIR. Characterization by XRD patterns in the disparate system of $\text{Ba}(\text{NO}_3)_2 : \text{KNO}_3$ show the existence of additional peaks and shift in peak positions corresponding to a new phase which indicate the configuration of solid solution. In the present distinct system $\text{Ba}(\text{NO}_3)_2 : \text{KNO}_3$ a marked increase in conductivity is found on introducing K^+ ion defects in a mixed system.

As well the presence of solid solution leads to the increase in entropy and subsequently increasing the concentration of more defects contributing to the enhancement of ionic conductivity. The effect of solid solution configuration can be either to insert or strengthen the physical property such as ionic conductivity. From FTIR also it is observed that new peaks and a shift in peak positions in the disparate system of $_{0.19}\text{Ba}(\text{NO}_3)_2 -_{0.81}\text{KNO}_3$ as compared with pure crystals i.e., $\text{Ba}(\text{NO}_3)_2$ and KNO_3 . This supports

the X-ray powder patterns in which we not only observed new peaks but also shift in peak positions of disparate crystals.

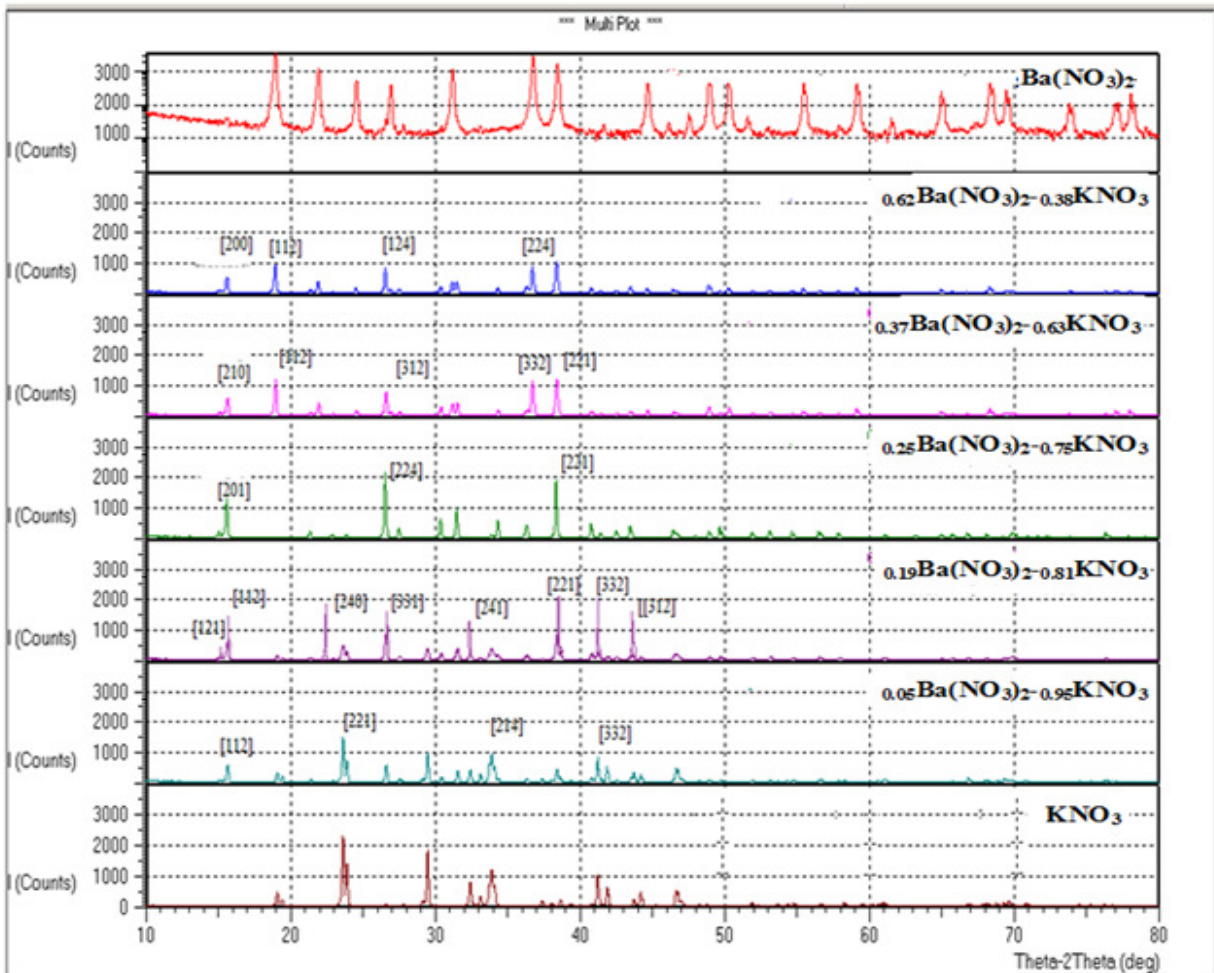


Fig.-1: XRD patterns for pure Ba(NO₃)₂ and KNO₃ and their Disparate Systems.

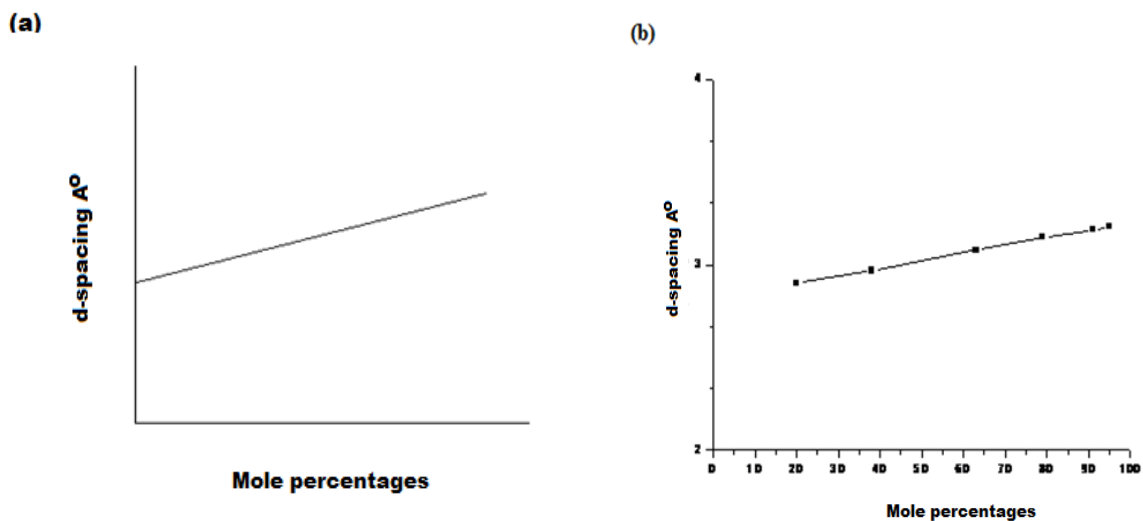


Fig.-2:(a) Schematic representation of ideal Vegard Behavior in a Li_{1+x}Ti_{2-x}Ga(PO₄)₃ system [Ref: 4]
 (b) In the present Disparate System (Ba(NO₃)₂ : KNO₃) showing ideal Vegard behavior.

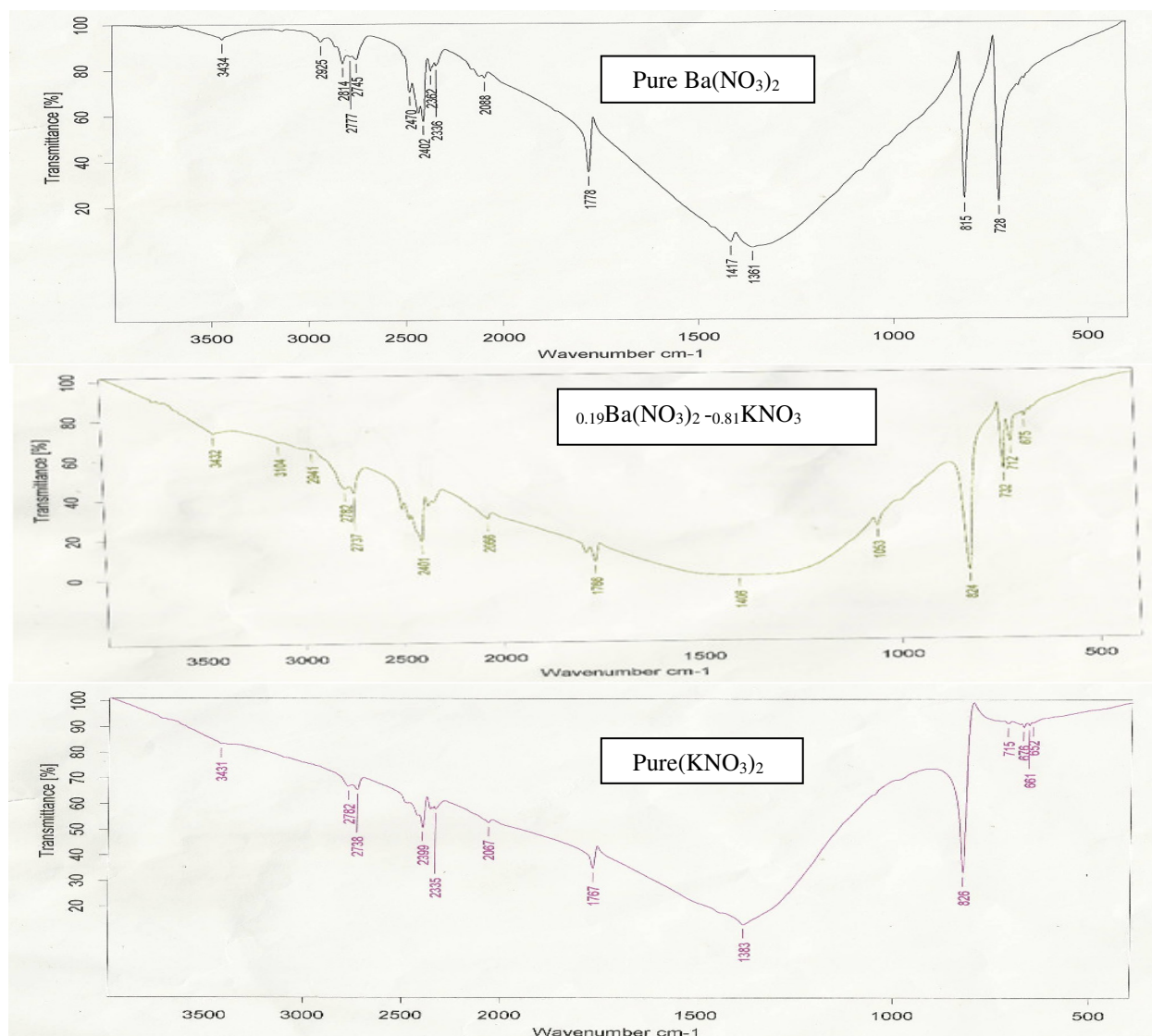


Fig.-3: FTIR patterns for pure $\text{Ba}(\text{NO}_3)_2$, KNO_3 and $0.19\text{Ba}(\text{NO}_3)_2 - 0.81\text{KNO}_3$ disparate System.

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