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Infrared Spectroscopy of Cupric Oxide Doped Barium Phosphate Glass.

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ABSTRACT

CuO powders were doped with barium phosphate glass with a series of $x\text{CuO}-(20-x)\text{BaO}-30\text{ZnO}-10\text{Na}_2\text{O}-40\text{P}_2\text{O}_5$ in molar ratio with ($x = 2, 4, 6, 8, 10$ and 12) were prepared by conventional quenching melts technique. FTIR transmission spectra have been carried out. The most active peaks were observed in the region from 450 cm^{-1} to 1700 cm^{-1} . FT-IR spectra were analyzed to determine and differentiate the various vibrational modes by applying a deconvolution method to the FT-IR spectra. The density has been measured by the conventional Archimedes method, molar volume were calculated and found the density and molar volume are trend in the same direction by increases the CuO contents.

Keywords: Absorption filter, Bandpass, Fourier Transform Infrared Spectra (FT-IR).

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INTRODUCTION

Glass science one of the most ancient techniques from the human kind, the developing of this science required for the new applications in the present era [1]. The most important commercial glass former are based on oxides for example silicate, borate, tellurite and phosphate [2]. The marvelous properties of phosphate glass such as low dispersion, high refractive index and low melting temperature compared to silicate glass [3]. The disadvantage of the phosphate glass such as chemical durability for the phosphate glass can be enhanced by doping with modifiers such as transition metals. The good modifier like transition metals oxide leads to increase the benefits of the glass with decreasing its chemical durability. Moreover, the fabrication of optical glass filter using BaO alkaline earth metal oxide has an effect on the improvement of devitrification resistance when it doped in small amount, but if we increase the amount of BaO the glass shows poor melting properties [4]. ZnO improvement the chemical durability, melting properties, and opacity of glass, which is very important for the optical properties for glass filter [5,6]. The oxide metals like zinc oxide playing a good rule for changing the properties of phosphate glass when it added as modifiers. The Zinc phosphate glass has significant interests because it exhibits a high durability, low melting temperature with a lower glass transition temperature, and glass forming ability. Zinc phosphate glass doped with copper ion were studied its structure by many techniques like XRD, NMR, XPS, [7-20].

In the present study, the physical properties such as FTIR infrared absorption spectra, density and molar volume were studied to examine the effect of copper oxide and barium oxide molar ratio on zinc phosphate glass for glass absorption filter applications.

EXPERIMENTAL

The glasses samples were prepared by copper oxide doped phosphate glass with a chemical composition $x\text{CuO}-(20-x)\text{BaO}-30\text{ZnO}-10\text{Na}_2\text{O}-40\text{P}_2\text{O}_5$ in molar ratio with ($x = 2, 4, 6, 8, 10$ and 12) applying the conventional melt and quenching technique. The starting materials were used as NaCO_3 , ZnO , $(\text{NH}_4)_2\text{H}_2\text{PO}_4$, and CuO . The chemical compositions were mixed and grinded using mortar for 30min for each sample, and then calcinated in porcelain crucible using muffle furnace for 1hour in 290°C to relieves the gases from the chemicals like CO_2 and NH_3 , after that the sample in the porcelain crucible replaced into melting furnace for 30min in 1100°C , then shaking in clockwise to ensure the material in high homogeneity. Finally, the casting quenched and annealed in copper mould with pressing plate to have a thin disk in temperature 300°C .

In this study we have some measurement to characterize the glass samples, FT-IR and density measured. FTIR infrared absorption spectra were carried out using the same weight of the glass powder dispersed in KBr pellets. The data were recorded by Perkin Elmer 457 spectrophotometer from 600 to 1700 cm^{-1} , the spectra were measured at room temperature with about 1cm^{-1} resolution for the instrument. A 1.0 mg from each sample was mixed with 100 mg of KBr in an agate mortar and pressed into pellets. The density of the glasses was measured by Archimedes' method, using ethanol as an immersion fluid at room temperature. Measurements were made in duplicate for each glass sample and the averages were taken. Molar volume was calculated from the density obtained. The density was measured by simple Archimedes method for all the glass samples using ethanol as an immersion liquid at room temperature. Molar volume was calculated from the density obtained.

RESULTS AND DISCUSSION

The infrared results of the glasses under investigation are shown in **Fig. 1**, where the spectra are shifted for the sake of clarity. The data has been drowning in such a way to get an idea about the replacement of BaO by CuO. In order to analyze the FT-IR absorption spectra, many trials have been done to deconvolute them using the Peak Fit computer program [21], at last it was found that the Gaussian band is the best fit. The only input for fitting program was the number of bands and the initial values for the parameters describing the intensity, position and width of each band. Subsequently, the program using a least-squares fitting procedure adjusted these parameters [22].

Fig. 2 shows, the FTIR spectra for glass 2 % of CuO along with the Peak Fit computer fitting in the wave number range from $1700 - 450\text{ cm}^{-1}$. There were no characteristic absorption bands in the region $> 1700\text{ cm}^{-1}$. The deconvolution bands of FT-IR spectra that studied glass yielded the central position, amplitude, area

and the full width at half maximum (FWHM) of each peak. The glasses show quite similar FT-IR spectra with slightly shifting to the position of the main peaks this due to the Cu^{2+} ions. The infra red absorption spectrum of CuO doped with barium phosphate glass **Fig. 2** the peaks at 1632 cm^{-1} reveals thermal vibrations of H^+ ions in an intermolecular phonon vibration associated with HPO_4^{2-} contacts. exhibited vibrational bands at 1287 cm^{-1} (identified duetoanti- symmetrical vibrations of PO_4^{3-} groups, this region may also consist of bands due to P=O stretching vibrations), 1082 cm^{-1} (a normal vibrationalmodein PO_4^{3-} group arising out of n^3 - symmetric stretching), 897 cm^{-1} (due to P–O–P asymmetric bending vibrations). This region may also consist of bands due to pyrophosphate groups ($\text{P}_2\text{O}_7^{4-}$). At 590 and 530 cm^{-1} P–O–H wagging and rocking vibrational bands are found [23-28]. Moreover, CuO shows three broad absorption peaks at 596 , 519 and 492 cm^{-1} , assigned to the stretching vibrations of Cu–O bond in the monoclinic CuO and the peaks observed in the absorption at 629 cm^{-1} which attributed to the stretching vibration of Cu–O vibration of the Cu_2O nanocrystals [29, 30]. Moreover, The Zn–O bond is assigned to the stretching frequency at 553 cm^{-1} [31].

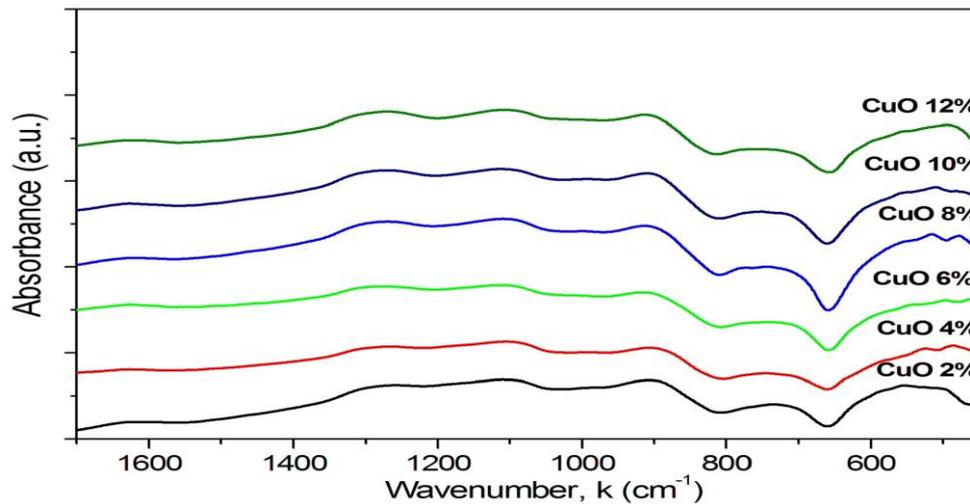


Figure 1: FTIR absorbance spectra of CuO nanopowders doped with barium phosphate glass

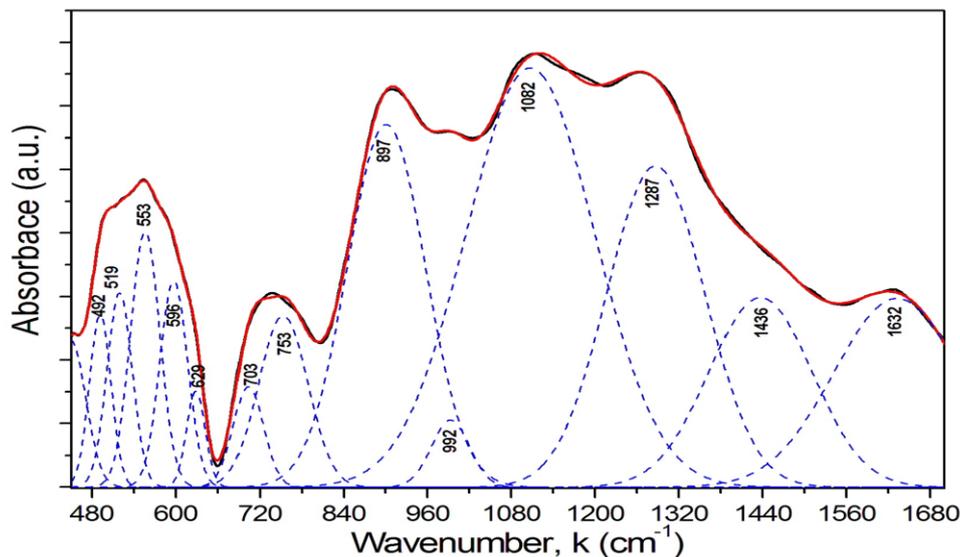


Figure 2: The band deconvolution of FT-IR spectra for glass of 2% CuO content in the spectral

The density and molar volume V_M were calculated according to relations [32]:

$$\rho = \left[\frac{W_{air}}{(W_{air} - W_l)} \right] \rho_0 \quad [1]$$

$$V_M = \frac{M_{W(glass)}}{\rho_{glass}} \quad [2]$$

Where ρ the sample density, ρ_0 the liquid density, W_{air} the weight in the air, W_l the weight in the liquid, V_M the molar volume and M_w the molar mass.

The density of the glass samples decreases as the barium contents decreases. Moreover, the molar volume and density decreases proportional to the barium content as shows in Fig. 3. The molar mass of barium oxide is heavier than the molar mass of copper oxide. So, the glass matrix with higher contents with barium oxide Ba^{2+} more dense. In addition, the decrease of molar volume is due to the atomic radius of Ba^{2+} higher than Cu^+ . As usually, the molar volume and density was changed with inverse direction of each other direction, but these unusual results. Inasmuch, BaO has high relative molecular mass which opens the structure of the glass network and introduces excess structure volume. CuO plays as a modifier, and by replacement of CuO by BaO causing decreases of overall molar volume [33-36].

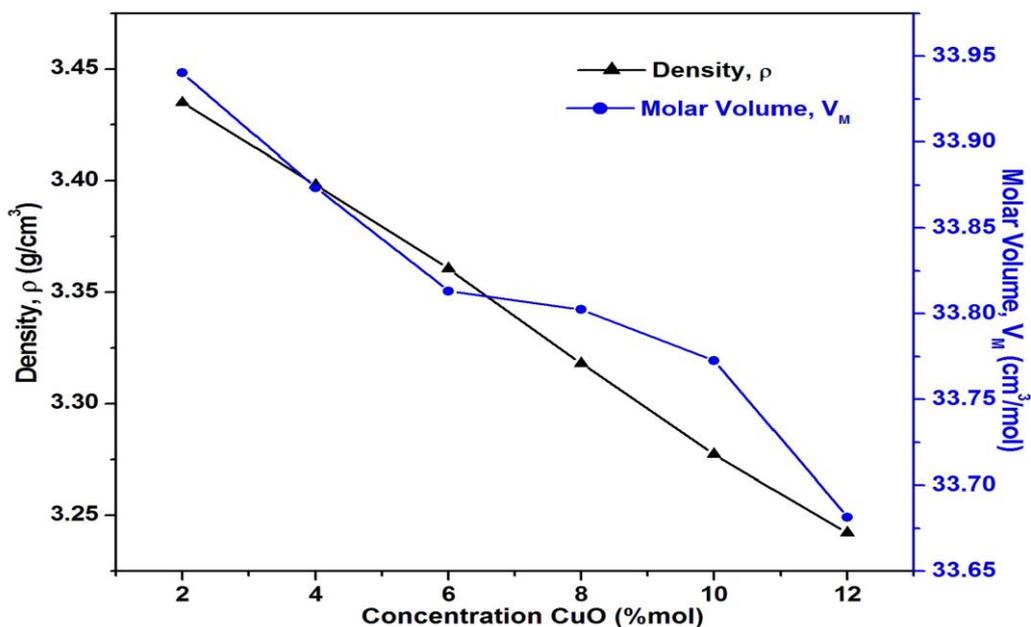


Figure 3: Density and molar volume as a function of CuO contents

CONCLUSION

The present study shows the effect of Cu ion of the barium phosphate glass, FTIR, molar volume and density were studies and describe the effect of Ba on the phosphate glass and the unusual increasing between the density and molar volume. The condensed units of BaO, which are the results of the molar ratio of CuO/BaO have an obvious effect on the infrared spectra at CuO = 2, 4, 6, 8, 10 and 12 mole %. The spectrum at CuO = 2 mole % might be controlled by the discrete ions of Cu^{2+} and barium phosphate glass.

Highlights

- The present study shows the effect of Cu^{2+} ion of the glass phosphate, Fourier transform infrared, molar volume and density on barium phosphate glass.
- Fourier transform infrared absorption spectra of cupric oxide doped barium phosphate glass exhibit the presence of several structural phosphate groups depending on the other cation partner

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