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Preparation and Structural Characterization of ZnO-Modified Sodium Phosphate Glasses: Density and Molar Volume Studies

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Abstract: Phosphate glasses have received considerable attention over the past several decades due to their distinctive properties and wide range of potential applications. Due to their lower melting and softening temperature, high electric conductivity and optical characteristic, phosphate glasses have been the subject of a large number of applications particularly in medicine, biology, optic, electronic [1,9,10]. Furthermore, alkali phosphate glasses have gained significant scientific interest due to their high ionic conductivity, relatively low melting temperature, and excellent glass-forming ability [1,9].

Ternary glasses of composition $42.5Na_2O:(57.5-x)P_2O_5:xZnO$ (x = 0, 0.5, 1, 2, 3, 4, and 5 mol%) were synthesized by the conventional melt-quenching technique. X-ray diffraction (XRD) confirmed the amorphous nature of all samples, evidenced by the absence of sharp crystalline peaks and the presence of broad diffuse humps in the 20–80° 2θ range. Density measurements, carried out using the Archimedes principle with benzene as the immersion liquid, revealed a systematic increase from 2.3075 to 2.4842 g/cm³ with increasing ZnO content, while the calculated molar volume decreased correspondingly from 46.786 to 42.239 cm³/mol. The oxygen-to-phosphorus (O/P) ratio increased from 2.8696 to 2.9524 across the series. These trends are discussed in terms of the network modifier/former role of ZnO in the sodium phosphate network, showing that the progressive incorporation of Zn^{2+} ions links the isolated phosphate tetrahedra, resulting in a more compact and polymerized glass network.

Keywords: *Sodium Phosphate Glass; ZnO; Melt Quenching; XRD; Density; Molar Volume.*

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I. INTRODUCTION

Phosphate glasses are of great technological interest due to their low melting temperatures, high thermal expansion coefficients, and unique optical properties [1, 2]. Unlike silicate glasses, which are built from a three-dimensional network of SiO4 tetrahedra, phosphate glasses consist of PO4 tetrahedra linked by bridging oxygens (BOs) in a chain-like structure [1, 3, 8]. The addition of network modifiers, such as alkali oxides (e.g., Na2O), breaks the P-O-P bridging bonds, forming non-bridging oxygens (NBOs) and depolymerizing the phosphate network [1, 3, 6]. This structural modification often decreases chemical durability and mechanical stability.

To overcome these limitations, the incorporation of divalent transition metal oxides, such as zinc oxide (ZnO), has been widely investigated [1, 2, 11]. Zinc oxide occupies a dual structural role in phosphate glass networks; it can act as a network modifier in octahedral coordination or as a network former in tetrahedral coordination [1, 11]. This structural flexibility allows ZnO to alter the network connectivity and physical properties, such as density and molar volume, in a systematic manner [1, 2].

Recent studies on zinc-doped phosphate glasses have demonstrated that substituting network formers with ZnO typically increases the density and decreases the molar volume of the glass network, indicating network contraction and structural compaction [1, 2]. For instance, Farag et al. [2] observed a systematic increase in density and contraction in molar volume in a sodium zinc phosphate glass-ceramic series, which they attributed to the formation of dense, cross-linked Zn-O-P structural units. Similarly, Refka Oueslati-Omrani et al. [1] demonstrated that ZnO

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incorporation enhances structural connectivity and density in silicate-phosphate glasses.

While several studies have explored the zinc-modified phosphate system [2, 4, 5], investigations into ultra-high alkali phosphate networks with compositions exceeding 40 mol% Na2O remain limited. In this work, the effect of ZnO substitution (0-5 mol%) for P2O5 in a high-alkali 42.5 mol% Na2O sodium phosphate base glass is systematically investigated. Through XRD, density, and molar volume measurements, we establish the physical and structural trends of this specific composition window, adding valuable data points and resolving critical physical trends in the literature.

II. EXPERIMENTAL

➢ *Materials and Method of Preparation*

High-purity (99.9%) Na_2CO_3, P_2O_5, and ZnO were used as starting materials. Glasses of composition $42.5Na_2O$:$(57.5-x)P_2O_5$:xZnO (x = 0, 0.5, 1, 2, 3, 4, 5 mol%) were prepared by the conventional melt-quenching technique. Batches of 10–15 g of the raw materials were weighed in the appropriate molar proportions using a monoplane balance, mixed thoroughly, and melted in a high-quality porcelain crucible in an electric furnace at a moderate heating rate, with the furnace temperature maintained approximately 20 K above the melting point (in the range 800–900°C) for 30 minutes. The homogenized melt was then quenched between two aluminium blocks to obtain clean, bubble-free, transparent glass samples approximately 2 cm in diameter and 0.1–0.2 cm thick, with no observable contamination from the aluminium blocks. Porcelain crucibles were used in preference to platinum to avoid extended cleaning times, with precautions taken to prevent crucible-derived impurities from entering the melt [7].

➢ *X-ray Diffraction (XRD)*

The amorphous nature of the as-quenched glasses was verified using a Seifert XRD 3003 T/T diffractometer with Cu Kα radiation (l = 1.541 Å) and a nickel filter, operated at an acceleration voltage of 40 kV and a tube current of 15 mA. A thick layer of powdered sample spread over a poly (methyl methacrylate) (PMMA) plate was used for recording the diffraction pattern. Diffraction patterns were recorded in reflection (Bragg–Brentano) geometry over a 2θ range of 20° to 80° in steps of 0.02°.

➢ *Density and Molar Volume*

Density was measured at room temperature by the Archimedes fluid-displacement method using benzene as the immersion liquid, with density calculated from:

$$\rho = \rho_b \times \frac{(M3 - M1)}{(M2 - M1) - (M4 - M3)} \quad (1)$$

where ρ_b is the density of benzene, and M_1–M_4 are the weights of the empty bottle, bottle + benzene, bottle + sample, and bottle + sample + benzene, respectively. Each reported value is the average of at least three independent measurements.

Measurements were conducted in triplicate to ensure an accuracy of ±0.0001 g/cm³. The molar volume (V_m) was calculated using the formula:

$$V_m = \frac{\sum xM}{\rho} = \frac{Mavg}{\rho} \quad (2)$$

where M and x represent the molecular weight and mole fraction of each oxide component, respectively, and M_{avg} is the average molecular weight of the glass series.

The oxygen-to-phosphorus (O/P) stoichiometry was mathematically calculated for each glass composition to monitor the concentration of network oxygen atoms relative to the glass-forming phosphorus cations.

III. RESULTS AND DISCUSSION

➢ *Structural (XRD) Analysis*

XRD patterns of representative compositions (Na 42.5%:P 54.5%: Zn 3%) show broad diffuse humps centered around 2θ » 25–30° with no sharp Bragg reflections, confirming the amorphous, long-range-disordered nature typical of oxide glasses. This is consistent with amorphous confirmation reported for ZnO-modified phosphate and related glass systems synthesized by the same melt-quench route [4,5].

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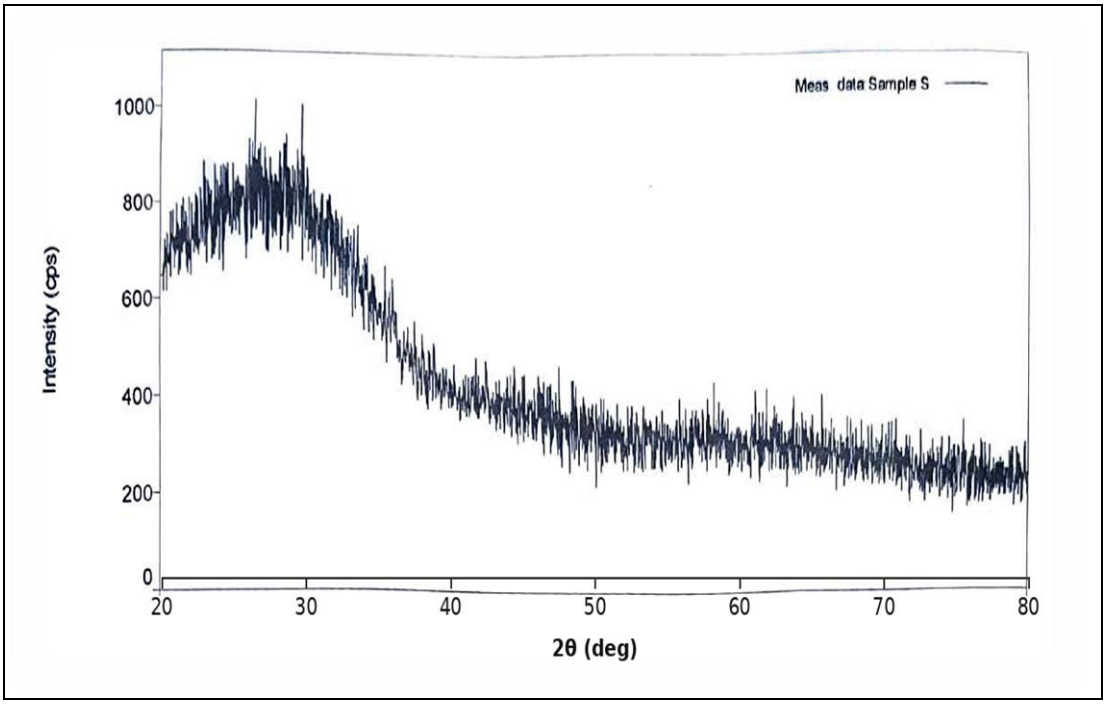

Fig 1. XRD Pattern of Sample Na 42.5%:P 54.5%: Zn 3%.

➢ *Density and Molar Volume*

Table 1. Density, Molar Volume, and O/P Ratio of 42.5Na_2O:(57.5-x) P_2O_5: xZnO Glasses as a Function of ZnO Content.

Composition (mol% ZnO)	***Density (gm/cm^3)***	***Molar Volume (cm^3/mol)***	***O/P Ratio***
0	2.3075	45.547	2.8696
0.5	2.3203	45.484	2.8772
1	2.3500	45.167	2.8849
2	2.3805	44.842	2.9009
3	2.4037	44.668	2.9174
4	2.4264	44.368	2.9345
5	2.4842	43.458	2.9529

The experimental density ρ and calculated molar volume (V_m) values for the glass series are 42.5Na_2O:(57.5-x)P_2O_5:xZnO (x = 0, 0.5, 1, 2, 3, 4, 5 mol%) tabulated in Table 1 as a function of ZnO concentration [1,3].

As observed, the glass density exhibits a monotonic increase from 2.3075 g/cm³ to 2.4842 g/cm³ as the ZnO content increases from 0 to 5 mol%. Concurrently, the molar volume (V_m) shows a systematic decrease from 46.786 cm³/mol to 42.239 cm³/mol across the same composition range. This systematic increase in density and corresponding decrease in molar volume indicate a significant contraction and structural compaction of the phosphate glass network [3,5].

This physical trend is dictated by two main structural factors –

➢ *Mass Effect:*

Although the formula weight of ZnO (81.38 g/mol) is lighter than that of a P_2O_5 formula unit (141.94 g/mol), the replacement of P_2O_5 by ZnO systematically alters the packing efficiency of the glass network [3,5].

➢ *Network Contraction and Polymerization:*

The Zn^{2+} cations possess a much higher ionic field strength 0.47$Å^{-2}$ compared to the dominant network modifier Na^+ 0.17 $Å^{-2}$ [10]. When ZnO replaces P_2O_5 in this high-alkali (42.5mol% Na_2O) matrix, the Zn^{2+} ions behave as cross-linking agents that link the isolated PO_4 tetrahedra via robust, partially covalent P–O–Zn linkages [3,11]. These P–O–Zn cross-links pull the terminal oxygen atoms closer together, effectively replacing the weaker, highly ionic, and open Na–O interstitial structure. This results in a tighter spatial distribution of the network-forming ions, which manifests physically as a structural contraction (revealed by the decreasing molar volume) and a highly compact glass network (reflected by the increasing density) [2,4,6].

This behavior is in excellent agreement with similar zinc-modified phosphate glass systems reported in the literature. For instance, Farag et al. [2] observed a systematic density increase and molar volume contraction in

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a sodium zinc phosphate glass-ceramic series, which they attributed to the formation of dense, cross-linked Zn–O–P structural units at the expense of terminal bonds. Similarly, Refka Oueslati-Omrani et al.[1] reported that incorporating ZnO into a sodium phosphate matrix significantly enhances structural connectivity and density, validating that the zinc-induced network compaction observed in this composition window reflects a general, non-anomalous structural response of the phosphate framework.

IV. CONCLUSION

Ternary $42.5Na_2O:(57.5-x)P_2O_5:xZnO$ glasses (x=0–5 mol%) were successfully synthesized by melt-quenching technique and confirmed to be amorphous by XRD. Density increased and molar volume decreased systematically with increasing ZnO substitution for P_2O_5, This behavior is attributed to progressive network contraction and structural compaction as Zn^{2+} ions successfully link the isolated phosphate tetrahedra, reducing the volume of the interstitial spaces and enhancing the overall network connectivity of the glass. These structural trends are consistent with, and add a new composition data-point to, the broader literature on ZnO-modified phosphate glass networks.

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