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A Significant Role of MoO$_3$ on the Optical, Thermal, and Radiation Shielding Characteristics of B$_2$O$_3$-P$_2$O$_5$-Li$_2$O Glasses

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ABSTRACT

Glasses based on borophosphate with the formula 42.5P$_2$O$_5$ – 42.5B$_2$O$_3$ – (15-x) Li$_2$O – xMoO$_3$ mol% where $x = (0 \leq x \geq 15)$ were manufactured using the melt-quenching methodology. The status of prepared samples was identified by (XRD). The temperature of the glass transition $T_g$, the temperature of onset glass crystallisation $T_c$ and the temperature of the crystallisation $T_p$ were evaluated using a differential thermal analyser (DTA). The energy gap ($E_{opt}$), Urbach ($E_u$), and parameters of dispersion were calculated through the data of optical spectra. Physical properties were determined and calculated, such as molar refractivity, metallization, electron polarizability, electronegativity, loss of reflection and dispersion parameters. Raising MoO$_3$ at the expense of Li$_2$O was used to assess the level of protection. For radiation protection applications, the glasses under investigation had superior characteristics.

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1. Introduction

B$_2$O$_3$-P$_2$O$_5$ glasses with superior efficiency can be used in a variety of different settings. Solid-state batteries, and nonlinear optics borophosphate glasses are appropriate. Due to its obvious advantages, lithium borophosphate is classical glass that has become recognized in storage batteries. These glasses are used as storage batteries in optical and electronic instruments. The addition of modifiers such as Li$_2$O influences of these characteristics. Li$_2$O will be combined instead of B-change BO$_4$ to BO$_3$ [1-8]. The characteristics of the combined glass (B$_2$O$_3$+P$_2$O$_5$) networks vary from those of the single glass B$_2$O$_3$ and P$_2$O$_5$ networks.

Transition metal oxides (TMOs) are a fascinating group of semiconductor materials because of their technological advantages for use in microelectronics and display systems. MoO$_3$ among (TMOs), due to its excellent use in optical materials and electrochemical devices has received increasing attention in recent years. There is a goal that support in manufacturing these glasses regarding the MoO$_3$ used in these implementations. Different MoO$_3$ preparation glasses were developed and investigated in response to this broad range of applications [9-16].

Due to the existence of MoO$_4$ and MoO$_6$ in the glass network, MoO$_3$ appears as the former non-conventional network. The existence of MoO$_3$ in glass systems does have a modifier impact on UV spectra [9-16]. There are increasingly diverse technologies for molybdenum borophosphate-based glasses, such as laser host fibers and superconducting switches.

Both scientifically and technologically, the significant advances of alkaline borophosphate glasses are considerable. The existence of PO$_4$ & BO$_4$ structural units, this consequence approaches from the structural issues connected with covalent links. In several fields, B$_2$O$_3$-P$_2$O$_5$ - Li$_2$O - MoO$_3$ glasses possess high applications because of their radiation shielding and good FT-IR transmission [17-33]. The object of this study is to assist you in the
preparation of $\text{B}_2\text{O}_3$-$\text{P}_2\text{O}_5$ - $\text{Li}_2\text{O}$ - $\text{MoO}_3$ glasses and investigating their optical and neutron shielding using Phy-X/PSD [34] properties.

2. Methodology

Table 1 shows how we formed the glasses in our published articles using the melt-quenching methodology. By melting together of $\text{B}_2\text{O}_3$ in its $\text{H}_3\text{BO}_4$ (Merck), $\text{Li}_2\text{O}$ in it $\text{Li}_2\text{CO}_3$ (Aldrich), $\text{P}_2\text{O}_5$ in it ($\text{NH}_4$)$_2\text{HPO}_4$ (Merck) and $\text{MoO}_3$ (Merck) in an open ceramic crucible. With the evaporation of CO$_2$, NH$_3$ and H$_2$O, $\text{Li}_2\text{CO}_3$, ($\text{NH}_4$)$_2\text{HPO}_4$ and H$_3\text{BO}_4$ and are converted into $\text{Li}_2\text{O}$, $\text{P}_2\text{O}_5$ and $\text{B}_2\text{O}_3$. The furnace temperature was changed at a melting temperature of 1050 °C. At 350 °C the prepared samples are annealed.

The Philips X-ray diffractometer (model PW / 1710) checked the condition of these glasses and glass-ceramics. The spectrophotometer was used to measure the optical spectra of the investigated glass system (type JASCO V- 670). The thermal investigation was carried out with a DTA-50 (Shimadzu-Japan). Phy-X / PSD can calculate a variety of shielding considerations [34]. Electron density ($N_{\text{eff}}$) was predictable as: $N_{\text{eff}} = N \frac{Z_{\text{eff}}}{\sum F_i A_i}$. Effective cross-section of removal ($\Sigma R$) projected as: $\left(\frac{\Sigma R}{p}\right) = \sum w_i \left(\frac{\Sigma R}{p}\right)_i$ and $R = \sum p_i \left(\frac{R}{p}\right)_i$. G–P fitting parameters has been predictable as $P = \frac{P_1(logZ_2-logZ_{\text{eq}})+Z_2(logZ_{\text{eq}}-logZ_1)}{logZ_2-logZ_1}$. EABF and EBF were predictable using G–P fitting $B(E,X) = 1 + \frac{b}{K-1}(K^x - 1)$ for $K \neq 1$, $B(E,X) = 1 + (b - 1)x$ $K = 1$ where $K(E, X) = cx^a + d \frac{\tanh\left(\frac{x}{X} - 2\right) - \tanh\left(-2\right)}{1 - \tanh\left(-2\right)}$.

3. Results and Discussion

3.1. XRD

Figure 1 depicts the glass system's X-ray features. In the glass samples, XRD revealed no discrete lines or sharp peaks, indicating a high degree of glass status.

3.2 Optical spectra
The absorption (A), transmittance (T), and reflectance (R) of glass samples are shown in Figures 2 and 3. Spectral UV according to reports, increasing. As a result, MoO$_3$ is to blame for the slight increase in BO [35-44]. Figure 4 shows the absorption coefficient of the glasses.

### 3.2.1 band gap $E_{opt}$

Glass spectrum in the UV and VIS areas were used for the estimated of the band gap energy $E_{opt}$ is estimated by $(\alpha \cdot h\nu)^{1/2} = B(h\nu - E_{opt})$ where B is an energy independent constant and $h\nu$ is photon energy. By intrigue the $(\alpha \cdot h\nu)^{1/2}$ versus $h\nu$ as Fig.5. Plot of $(\alpha \cdot h\nu)^{1/2}$ against photon energy ($h\nu$) to evaluate the indirect $E_{opt}$ from the intercept. $E_{opt}$ increases with increasing MoO$_3$, as revealed in Table 2, due to oxygen bridges (BO) form and bind excited electrons more tightly than non-bridging oxygen electrons (NBO). Urbach energy has been calculated $\propto \exp\left(\frac{h\nu}{E_u}\right)$, Fig. 6 and table 2 show that their $E_{opt}$ values have an inverse relationship. The values of $E_{opt}$ and $E_u$ was shown in Fig.7.

The refractive index was calculated using: $n = \frac{(1-R)^2 + k^2}{(1+R)^2 + k^2}$ where $k = \alpha \lambda / 4\pi$. The refractive index presented in Fig.8 for fabricated glasses. It has already been stated that density increase, the refractive index of these samples increased. As a result, it can be directly compared to reflectance and density, and opposite to molar volume.

### 3.2.2 Dispersion parameters

As approximated, molar polarization and polarizability of glasses were computed:

$$R_m = (n^2 - 1)n^2 + 2\gamma m, \quad \alpha_m = (3|4\pi N|)R_m, \quad \text{and} \quad \alpha_0^2 = \frac{\gamma m(n^2 - 1)n^2 + 2\gamma m}{N\alpha^2 - \sum_{cat}}$$

Polarization was linked with the optical basicity; $\Lambda = 1.67\left(1 - \frac{1}{\alpha^2}\right)$. Figs. 9,10& 11 exemplifies the polarizabilities, Molar Polarizability $\alpha_m$ and optical basicity separately of the
samples. The refractive index is trending in the same direction with MoO$_3$ content has been reported to enhance.

The molar refractivity as $E_{opt}$. $R_m = Vm\left(1 - \sqrt{E_g/20}\right)$ and molar polarizability ($\alpha_m$) $\alpha_m = \left(\frac{3}{4\pi N}\right)R_m$. Reflection loss $R_L = \left(\frac{R_m}{Vm}\right)$. Because the molar volume decreases with Mo$^+$, these values of ($R_m$) ($\alpha_m$) and ($R_L$) decline. The criterion for metallization is predicted as $M = 1 - \frac{R_m}{Vm}$, the metallization value increase with Mo$^+$. The electronegativity ($\chi$) is predicted as $\chi = 0.2688E_{opt}$. where $E_{opt}$ bandgap. Thus, with Mo$^+$ increasing, the electronegativity ($\chi$) values increase. The electron polarizability is predicted as, $\propto° = -0.9\chi + 3.5$ and optical basicity $\wedge = -0.5\chi + 1.7$. $\propto°$ and $\wedge$ have the opposite value of ($\chi$) so, $\propto°$ and $\wedge$ decrease with Mo$^+$. These items are obtainable in Table 2.

The dispersion was calculated by Wemple and Didomenico $E_o$ and $E_d$ [50-53]. The hypnosis designates explained by $n^2 - 1 = \frac{E_o}{E_o - E^2}$ [64-70]. The plotting of, ($n^2$-1)$^{-1}$ with (hu)$^2$ $E_o$ and $E_d$ predictable from the slope and intercept as shown in Figs. 12 & 13. It mentioned that with increasing MoO$_3$, $E_o$ and $E_d$ were slightly enhanced. The optical energy $E_{opt}$ that represent $E_{opt} = \frac{E_d}{2}$. Refractive Static index at infinite wavelength ($n_o$) was estimated by $n_o = \sqrt{1 + \frac{E_d}{E_o}}$ and the static dielectric $\varepsilon_{\infty} = n_o^2$. The oscillator's wavelength ($\lambda_o$) and strength ($S_o$) were calculated using the following formula $n^2 - 1 = \frac{S_o \lambda_o^2}{1-(\frac{\lambda}{\lambda})^2}$. These items are obtainable in Table 3.

3.3 DTA

The thermal analysis (DTA) of glass samples demonstrated in Fig. 14. The temperature of the glass transition, $T_g$, is 493-532 ±3 °C. The temperature of the glass crystallisation $T_c$ starts at 537-580 ±3 °C. The temperature of the glass crystallisation $T_c$ ends at 606-645 ±3 °C. According to DTA observations, $T_g$ increases from 493 into 532 °C, $T_c$ increases from 537
into 580 °C and Tp increases from 606 into 645 °C with the increase of MoO₃ content. The transformation of Li-O to Mo-O linkages is significantly associated with this behaviour. Hence, Li−Li (137.3±6.3 KJ/mol) dissociation energy is weaker than Mo−Mo (449.4±1 KJ/mol) dissociation energy and adding MoO₃ variations the basic B units from BO₃ to BO₄. Thermal stability estimated by \( \Delta T = (T_c - T_g) \), weighted thermal stability \( H_g = \Delta T / T_g \) and \( S = (T_p - T_c) \Delta T / T_g \). It observed that all thermal stability of samples improved as MoO₃. The \( T_g, T_c, T_p \) and thermal stability values are obtainable in Table 4.

### 3.4 Photon Shielding Features

The level of protection was assessed in this article by increasing MoO₃ at the expense of Li₂O with the composition 42.5B₂O₃ – 42.5P₂O₅ – (15 − \( x \) )Li₂O – \( x \) MoO₃, \( 0 \leq x \geq 15 \). The mean free path (MFP) is depicted in Fig.15. It was stated that as photon energy increases, the values of (MFP) increase. This insight revealed that as the photon's energy increases, it becomes capable of transmitting samples on purpose. Because the lower value of the (MFP) sample has a higher MoO₃ content, good radiation attenuation glasses are available.\[54-71\].

Figure 16 demonstrations the \( (N_{eff}) \) of fabricated glasses. It is demonstrated that \( (N_{eff}) \) decreases and then rises as energy increases. This significant decrease can be attributed to the interaction of Compton scattering. The effect of forming pairs at higher energy levels as MoO₃ is linked to the increasing in \( (N_{eff}) \).

The ASC of fabricated glasses are presented in Fig. 17. The ASC and ESC values are expected to decrease as energy rates increase. This decrease occurs due to the Compton scattering interaction. The \( C_{eff} \) of fabricated glasses depicted in Figure 18. With the increase in photon energy, it is predicted that \( C_{eff} \) will decrease. The impact of pair-creation was reflected in the increase in \( C_{eff} \).
The EBF & EABF of fabricated glasses were characterized by Figs. 19&20. EBF and EABF values are determined by the lower energy and concentration of the glass samples. At lower energy levels, EBF and EABF values are low, but they rise as energy levels rise. After that, gradually decrease as energy level rises. So, we can divide the energy scale into three parts low, medium, and high. The first part (low energy): the typical phase is the photoelectric effect, and the relationship is reversed with light, and the glasses will absorb the energy photons. The photons are therefore not allowed to build-up. In the second part (medium energy): the common process is the Compton scattering, the values of EBF and, EABF is increased in all samples independent from the MFP. Through this part, the photons stay in the samples for a long time, as these processes lead to high accumulation value due to multiple scattering processes. Third parts (high energy): the common process is the pair production. In this process, EBF and, EABF is decreased with energy. Therefore, these data helped in the determination of maximum radiation intensity occur. In this research, highest radiation occurs on the surface of the sample. In Fig. 21, fast cross section neutron removal (FNRCS) is shown. It was stated that MoO3 improved FNRCS.

4. Conclusions

In the existing research, molybdenum lithium borophosphate glasses $42.5P_2O_5 − 42.5B_2O_3 − (15-x) Li_2O − xMoO_3$ where $x = (0 \leq x \geq 15)$ were fabricated with conventional melt-quenching procedures. The optical, thermal, and shielding factors were observed. The findings showed the following objects:

1- Because of the increase in MoO$_3$, the metallization of these glasses was improved.

2- The 2.23 for G 1, 2.32 for G 2, 2.38 for G 3, 2.41 for G 4, and 2.49 for G 5 were identified as the indirect optical bands that were collected.

3- Urbach energies of these samples were reduces as the content of MoO$_3$ increase.

4- As the density of the investigated glasses rises, the refractive index rises as well.
5- These glasses were investigated for molar polarization, polarizability, and optical basicity.

6- $T_g$, $T_c$, $T_p$ and thermal stability values are enhanced with MoO$_3$.

7- The fabricated samples' gamma shielding features were predictable. The impact of adding MoO$_3$ to the glasses on their shielding ability was mentioned.

8- Lower value of the (MFP) sample has more MoO$_3$ are good radiation attenuation glasses are available.

9- As the concentration of MoO$_3$ increased, these glasses have a high cross section neutron removal rate.

The findings discovered that as MoO$_3$ increase the glass system can result in significant improvements in attenuation and optical characteristics. Furthermore, it is possible to use this glass in optoelectronic, optical devices, and a radiation shield for use in x-ray centers.
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Figures

Figure 1

XRD of the studied glasses.
Figure 2

The absorbance (A) and Transmittance (T) of the prepared glasses.

Figure 3

The reflectance (R) of the prepared glasses.
Figure 4

The absorption coefficient of the prepared glasses.

Figure 5

Plot of \((\alpha \nu)^{1/2}\) against photon energy \((\hbar \nu)\) to calculate the indirect optical band gap from the intercept of the curves.
Figure 6
Dependence of $\ln(\alpha)$ upon the photon energy ($h\nu$) for the prepared glasses.

Figure 7
Optical band gap and Urbach energy versus concentration of MoO$_3$. 
Figure 8
Refractive index of the prepared glasses.

Figure 9
Molar refractivity of the prepared glasses.
Figure 10

Electronic polarizability of the prepared glasses.

Figure 11
Optical basicity of the prepared glasses.

Figure 12

Variation of $(n^2 - 1)^{-1}$ with $(h \nu)^2$ for the prepared glasses.
Figure 13

Variation of \((n^2 - 1) - 1\) with \(1/(hu)\) for the prepared glasses.

![Graph showing variation of \((n^2 - 1) - 1\) with \(1/(hu)\) for prepared glasses.]

Figure 14

DTA of the prepared glasses.
Figure 15
The MFP for the prepared glasses as a function of photon energy.

Figure 16
The $\text{(Neff)}$ for the prepared glasses as a function of photon energy.

Figure 17

The ASC for the prepared glasses as a function of photon energy

Figure 18
The $C_{\text{eff}}$ for the prepared glasses as a function of photon energy.

Figure 19

Variation of EBF versus the gamma ray energy for the prepared glasses as a function of photon energy.
Figure 20

Variation of EABF versus the gamma ray energy for the prepared glasses as a function of photon energy.
Figure 21

FNRCs for the prepared glasses comparison with standard materials.