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Title of Thesis: Structure, Optical, Mechanical and Shielding properties of Oxy-fluoride glass system

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ABSTRACT

This study investigates the influence of increasing PbF2 concentration on the physical, optical, mechanical, and radiation shielding properties of a proposed oxy-fluoride glass system xPbF2:10 CaO:20 Na2O:(70-x) B2O3, where x ranges between 0 and 25 mol.%. Melt quenching techniques were used to prepare six distinct samples, tagged as BPbF0, BPbF5, BPbF10, BPbF15, BPbF20, and BPbF25.

The density, molar volume, and oxygen packing density increase as the PbF2 content increases, .indicating the formation of non-bridging oxygen atoms and the expansion of the glass network

The produced glass samples were subjected to x-ray diffraction (XRD) and Fourier Transform Infrared (FTIR) tests to explore the effect of increasing the concentration of lead-fluoride PbF2 on the structural. The absence of crystalline peaks in X-ray diffraction (XRD) spectra confirms the glassy nature of the prepared glass samples. The FTIR method was used to evaluate the impact of PbF2 on the structural properties of the produced glass system. It has been discovered that lead fluoride acts as a modifier, converting triangular [BO3] units to tetrahedral [BO4] units, as well as forming non-bridging .oxygen and increasing ionic character

An ultraviolet-visible (UV-Vis/NIR) spectrophotometer was used to evaluate optical properties. Optical measurements show that the refractive index increases and the indirect band gap energy decreases with increasing PbF2 concentration. This increment may be ascribed to the rise in glass density and the formation of non-bridging oxygen atoms (NBO). . The metallization constant M values are in the range of ($0.407 \leq M \leq 0.434$), this confirms the insulating nature of the prepared glass samples. The values of the electron negativity (χ), the electronic polarizability (∝_o), and the optical basicity (Λ) were determined and it show increase in the electronic polarizability (∝o), and the optical basicity (Λ)with increasing the PbF2 content. This trend suggests a potential increase in electron .localization

The Bond Compression (BC) model was used to investigate the mechanical properties It was found that, increasing PbF2 concentration leads to an increase in the average cross-link density ($\overline{(n_c)}$), an increase in the number of lattice bonds per unit volume of glass (n_b), a decrease in both the average bond stretching force constant ($\bar{F}$) and the average atomic ring size (l) decrease. There is also a slight .decrease in elastic moduli and an increasing in the hardness

Furthermore, using the Phys-X/PSD software, the gamma radiation shielding parameters such as the linear attenuation coefficient (μ), half-value layer thickness (HVL), mean free path length (MFP), effective atomic number (Zeff), effective electron density (Neff), exposure buildup factor (EBF), and energy absorption buildup factor (EABF) were theoretically calculated. Furthermore, using the NGCAL software, the effective macroscopic cross section for 0.0254eV thermal and 4MeV fast neutrons was calculated. The results demonstrated that raising the PbF2 content increases the radiation shielding properties of the glass samples under consideration. As a result, the BPbF25 sample absorbs more gamma and fast neutrons than the other samples in our investigation.

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