Investigation of Lead borate glasses doped with Mn^{2+}: Comprehensive analysis of radiation shielding properties

K. Chandra Sekhar[1], R. Umamaheswara Singh[2], G. Nagaraju[3], R. Nagaraju[4], Md. Shareefuddin[5]*

[1]Department of Physics, University College of Science Saifabad, Osmania University, Hyderabad, Telangana, 500004, India
[2]Department of Physics, Hyderabad Institute of Technology and Management, Hyderabad, Telangana, 501401, India
[3]Department of Physics, Government Degree College (A), Khairatabad, Hyderabad, Telangana, 500004, India
[4]Department of Physics, Vasavi College of Engineering, Hyderabad, Telangana, 500031, India
[5]Department of Physics, Osmania University, Hyderabad, Telangana, 500007, India

Abstract. Lead oxide (PbO) is a crucial component of borate glasses despite its toxicity because its presence significantly enhances their characteristics for specific uses, like radiation shielding and optical devices. The present work deals with the radiation shielding features of the borate glasses containing high density chemicals (PbO & $PbCl_2$). The glasses with composition $xPbCl_2$–(30 − x)PbO–69.5B_2O_3–0.5MnO_2 with $5 \leq x \leq 25$ mol% were prepared using melt quenching method. To obtain the shielding characteristic of samples like MAC, LAC, Z_{eff}, etc., the well-known and reputable Phy-X/PSD online tool is utilized. The data flattened on the higher energy side (CE and PP) and showed increased MAC and LAC in the lower energy (PE) region. Lower concentrations of $PbCl_2$ demonstrated better LAC and MAC since sample density diminished as $PbCl_2$ increased.

1 Introduction

The latest developments in nuclear power technology have heightened human exposure to radiation that causes ionization. Given that prolonged exposure to radiation adversely affects human health, the development of novel materials that mitigate radiation risks is crucial. Conventional protection from radiation substances possess advantages and disadvantages. Gamma-ray shielding often employs materials with large atomic numbers. Lead is favored due to its substantial density and ability to attenuate radiation. Concrete composed of water, cement, and aggregate is robust and economical [1, 2]. Lead borate glasses are compelling systems for examining the link between design, composition, and properties of glasses. They display extensive glass-forming areas and demonstrate considerable diversity in atomic structure based on content. Moreover, spectroscopic analyses of these sorts of glasses are

* Corresponding author: chandu9417@gmail.com

advantageous due to the significant disparity in mass between lead and boron atoms, which facilitates the differentiation of vibrational modes of PbO polyhedra and the borate framework. These glasses possess technical importance due to their ability to demonstrate zero stress optic characteristics and improved optical non-linearity. The interplay within the chemical makeup and the framework of lead borate glasses reveals intriguing characteristics, as lead functions either as a glass creator or modifier contingent upon the composition [3 - 5]. Mn^{2+} ions are the vital elements of lead borate glasses, and they are responsible for determining the structural, optical, and electrical properties of the material. The dual role that they play in the glass network and the distinctive spectroscopic fingerprints that they possess are the primary factors that determine their significance. Recent studies have shown that the presence of Mn^{2+} ions in lead borate glass systems significantly enhances their radiation shielding qualities [6, 7]. This is accomplished by boosting the linear and mass attenuation coefficients, which in turn makes these systems suitable for deployment in photon shielding purposes.

In contrast to complicated lab tests or other simulation programs, Phy-X/PSD software offers a fast, inexpensive, and easy-to-use method of calculating essential parameters (such as MAC, LAC, HVL, etc.) for any kind of material across a broad range of energies (1 keV - 100 GeV). This allows for the rapid assessment and advancement of shielding substances for X-rays and gamma rays, reducing precious resources and time. Phy-X/PSD is a robust and user-friendly digital instrument for the swift assessment and enhancement of radiation shielding materials, rendering it essential for contemporary radiation safety [8 - 11].

2. Experimental

2.1. Sample preparation

One of the simpler methods that was used to prepare the glass samples is melt quenching method. For the preparation of the samples the chemical formula used is $xPbCl_2$– (30 − x) PbO–$69.5B_2O_3$–$0.5MnO_2$ with $5 \leq x \leq 25$ mol% coded as PCPBM-1, PCPBM-2, PCPBM-3, PCPBM-4 and PCPBM-5. The present glass samples were made using high pure chemicals boric acid (H_3BO_3), lead chloride ($PbCl_2$), lead oxide (PbO), and Manganese Oxide (MnO_2). The content of lead chloride increased and lead oxide decreased in steps of 5 mole while the other two components maintained constantly. Following the precise measurement and mixing of these ingredients, they were subsequently placed in an electric furnace for forty minutes at a temperature of around one thousand degrees Celsius. It was then necessary for stirring the liquid in order to guarantee that the bubbles were released. For the purpose of to reduce the amount of mechanical stress, we carried out the annealing process in another furnace at a temperature of 250^0 degrees Celsius for around three hours. We cooled the furnace at a rate of 200 degrees Celsius per minute in order to get the temperature down to a level that was closer to the ambient temperature.

2.2. Characterization

The law of Archimedes was utilized to ascertain the density of PCPBM glasses, using xylene as the immersion solvent. Three unique specimens were chosen from every single glass sample for density assessment, and the mean value has been documented as the final density for every single sample. When it comes to determining the shielding capability of glass samples based on density and chemical composition, the Phy-X/PSD software is an extremely helpful piece of software that can be found as a free download on the internet. Additionally, this program was helpful in overcoming the restrictions of the laboratory in order to assess the shielding efficacy of the materials by using them. Because radiation processes involve photon energies ranging from 0.015 to 15 MeV, the programme that was built evaluates the capacity to shield between these energies. When the glasses were subjected to radiation of the requisite photon energy range, the program which was used to determine the various shielding properties of the glasses was used. The data that is obtained through the utilization of this software is of a high level of accuracy, with a variance of ±5%. This data is gathered from many simulations and theoretical calculations, as indicated by the references provided. The gamma ray protection of the glasses assessed with the parameters (MAC, LAC, HVL etc) which were determined by using Phy-X/PSD software for the prepared glass samples.

3. Results and discussion

3.1. Density and molar volume

The density of glass affects its ability to withstand stress and collisions, consequently preserving the integrity of its framework. Density is a crucial element in industrial and production environments, as it affects the effectiveness and utility of glass for numerous purposes.

Table 1 Glass composition in mol%, density and molar volume of the PCPBM glasses

Glass Code	Chemicals in mol%				Density (ρ) (g/cc)	Molar Volume (V_m) cc/mol
	$PbCl_2$	PbO	B_2O_3	MnO_2		
PCPBM-1	5	25	69.5	0.5	4.530	34.45
PCPBM-2	10	20	69.5	0.5	4.181	37.98
PCPBM-3	15	15	69.5	0.5	3.720	43.31
PCPBM-4	20	10	69.5	0.5	3.511	46.80
PCPBM-5	25	5	69.5	0.5	3.021	55.29

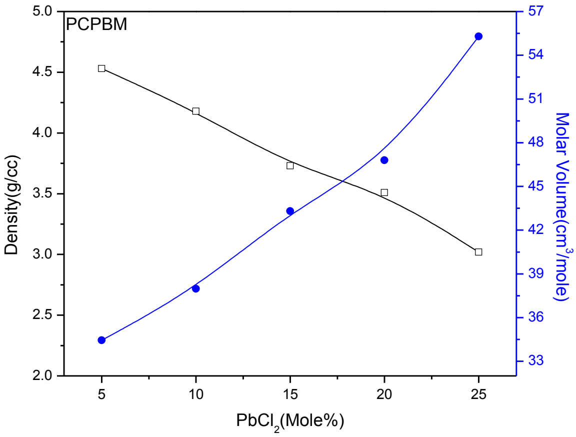

Fig. 1 Change in density and molar volume with $PbCl_2$ content

Glass samples are assessed by density evaluations, and it is unlikely that two specimens from an identical origin emanated from the identical area if the density of them differ markedly. In samples with numerous shards, measurement of density can function as an assessment tool to discern different glass sources involved [12. 13]. The chemical composition and density values shown in table 1. The density values of the PCPBM-1-PCPBM-5 samples are 4.530, 4.181, 3.720, 3.511, and 3.021 g/cc (can be seen in Fig 1). In this case, the density was found to be reducing as the $PbCl_2$ concentration increased, whereas the molar volume improved. In the PCPBM glass system, the increase of PbCl2 corresponds to a proportional decrease in PbO, indicating that chlorine is substituting for oxygen within the glass matrix. The rising molar volume results from the larger ionic radii of chlorine (1.81 Å) ions in contrast to oxygen (1.40 Å) ions. Chlorine ions fill greater amounts of space over oxygen and can additionally occupy interstitial spaces in the glass network, resulting in reduced density and increased molar volume in PCPBM glasses. The incorporation of chlorine likely enlarges the glass network, thereby diminishing its structural integrity. The aforementioned factors may be ascribed to the rise in molar volume of the current PCPBM glass samples. The density and molar volume values are determined to be in reasonable agreement with the given values [14, 15].

3.2. Gamma ray shielding quantities

MAC and LAC values were obtained from Phy-x/PSD software The mass attenuation coefficient, also known as MAC, is a fundamental parameter that quantifies the resistance of a material to the transmission of gamma and x-rays through it.

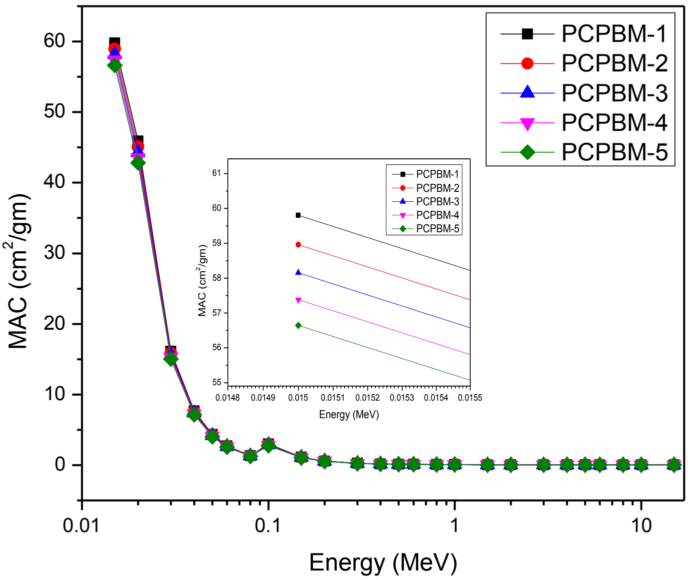

Fig. 2 Variation of MAC with energy in PCPBM glasses

It is common practice to utilize the knowledge of μ_m in order to determine the capacity of a medium to act as a radiation absorber or shield, or for the purpose of conducting dosimetry experiments. Phy-X software was utilized in order to ascertain the MAC value of the glass samples that had been created. The data (Fig 2) demonstrates that the glass sample with the PCPBM-2-PCPBM-5 code has the lowest MAC, which varies from 0.038-58.962, 0.038-58.155, 0.038-57.383, and 0.037 to 56.644 cm^2 g^{-1} respectively for gamma photon energies ranging from 0.015 to 15 MeV [16]. The glass sample with the PCPBM-1 code has the highest MAC, which increased from 0.038 to 59.806 cm^2 g^{-1}. According to the findings, the sample that contains a greater quantity of PbO has a considerably higher attenuation coefficient.

When it comes to determining the extent to which a sample can protect itself from ionizing radiation, the LAC is one of the most important measures that is used. The explanation and plotting of the linear attenuation coefficient μ for the S1 to S5 glass samples can be found in figure (3) respectively. According to Beer-Lambert's law, the LAC value has a maximum value of 15 KeV for the PCPBM-1 to PCPBM-5 glasses, which resulted in a change from 270.923 cm-1 to 171.120 cm-1 [17]. The data on the physical attributes reveals that PCPBM-1, which has a high PbO content, has the maximum density in comparison to other samples. As a result, it is an excellent shielding material that has a high attenuation coefficient. The sample that has a low amount of lead oxide has a low density and a reduced LAC value.

The observed pattern can be explained by the fact that lead has a stronger molecular weight, density, and atomic number in comparison to the other elements that are present in B2O3. Given that the probability of photon interaction rises with increasing atomic number, it follows that the heavier lead (Pb) atom is exposed to a greater quantity of photons than either the boron (B) or oxygen (O) atoms were. It is [18]. As the photon energy grows as a result of the photoelectric effect and Compton Scattering, the LAC value drops dramatically, however there is a tiny increase recorded above 6 MeV as a result of pair production. It is [19]. In the PCPBM-1-PCPBM-5 samples, the μ value is found to be low at 6 MeV, with values of 0.158, 0.145, 0.129, 0.121, and 0.104 cm-1 on a respective basis. The sudden spike in LAC that was discovered at 0.1 MeV was revealed to be caused by the K absorption edge of the heavy component Pb, as was determined by the investigation. In addition, this finding was attained by utilizing a variety of glasses containing lead. [20].

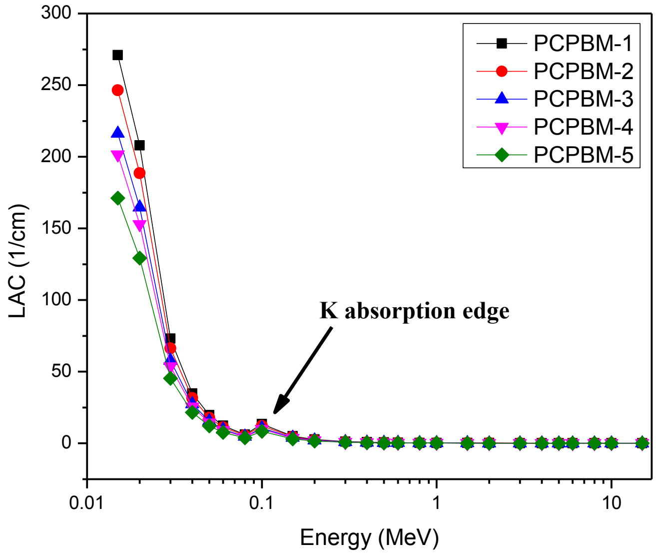

Fig. 3 Variation of LAC with energy in PCPBM glasses

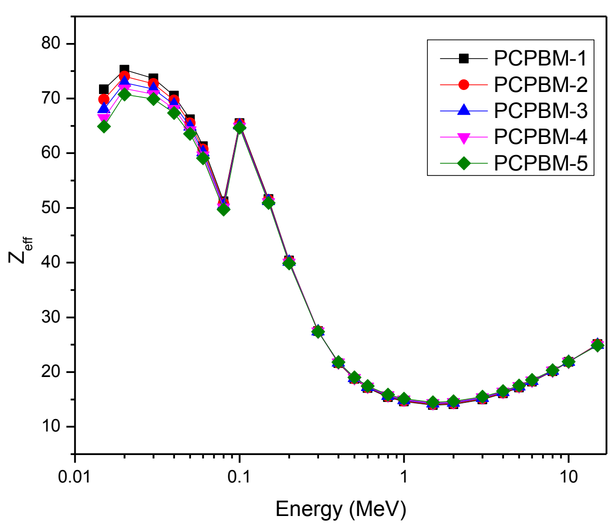

Fig. 4 Variation of Z_{eff} with energy in PCPBM glasses

Effective atomic number Z_{eff} is one of the major shielding characteristics for multi-element materials, and the data reveal that it fluctuates with energy and is affected by the collision

mechanism that is implicated. Z_{eff}, which stands for the effective number of electrons for photon interactions, varied throughout the samples as the incident photon energy changed. For present glass samples of PCPBM-1-PCPBM-5 maximum Z_{eff} value varies from 71.67 to 13.94, 69.79 to 14.08, 68.05 to 14.22, 66.41 to 14.35 and 64.88 to 14.49 respectively. An illustration of these variances can be found in figure (4). To a large extent, the energy response of the Zeff follows a trend that is nearly identical to that of the attenuation coefficients. The fact that it grows corresponds to the fact that the quantity of lead that can be found in the glasses rises, which results in the rise in density [4, 11]. According to the outcomes, one may reach the opinion that the sample having a high density had adequate transparency and might therefore be useful for purposes requiring radiation shielding.
When it comes to shielding concepts, it is frequently easiest to define the photon penetration efficiency of a medium through the half value thickness (HVL). One of the most important aspects of HVL is that it provides substances with a capacity to shield. It is a measure of the thickness of the protective layer that permits fifty percent of the photon that is impinge on the substance to pass across it[21, 22]. Fig. (5) shows the Half Value Layer variation with photon energy for the PCPBM-1-PCPBM-5 glasses. Due to inverse relation between μ and HVL, graph showing opposite pattern to LAC graph. The HVL is 0.003 to 0.004 at 15 KeV for PCPBM-1-PCPBM-5 glasses, have small value. At 6 MeV all the samples possess highest HVL values for PCPBM-1-PCPBM-5as 4.389, 4.774, 5.387, 5.729 and 6.681 respectively. From the data it is concluded that with less HVL value compared to other samples, S1 sample which consist high PbO content has become good shielding material.

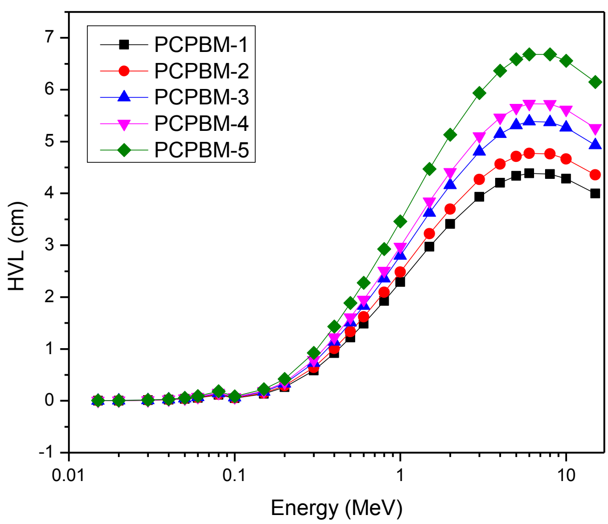

Fig. 5 Variation of HVL with energy in PCPBM glasses

This figure depicts the Mean Free Path (MFP) of the samples that were processed and plotted as indicated in figure 6. According to the findings, the MFP values of the samples range from 0.004 to 0.006 for PCPBM-1-PCPBM-5 when measured at 15 KeV of energy. The MFP value increases as the photon energy increases, and it reaches its highest value at 6 MeV, which is 6.332, 6.888, 7.771, 8.265 and 9.639 for PCPBM-1-PCPBM-5 samples, respectively. According to the findings, the PCPBM-1 sample, which has a high density and a low MFP value, has the potential to be the most effective shielding material..

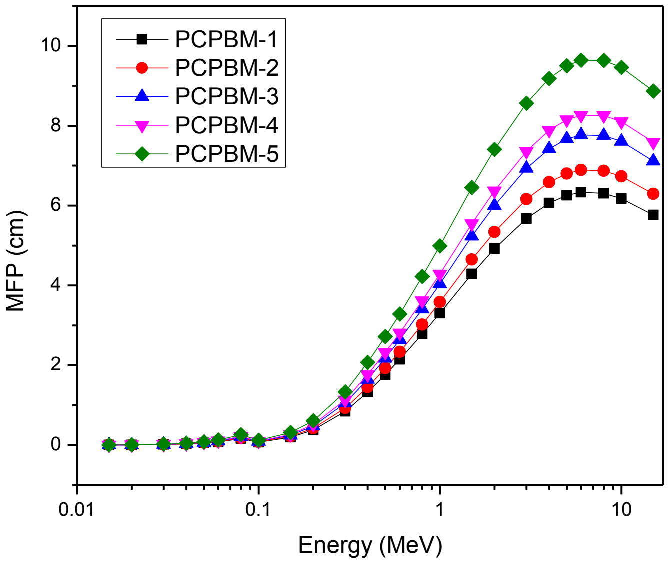

Fig. 6 Variation of MFP with energy in PCPBM glasses

4. Conclusions

The present study consists of five PCPBM samples that were generated by employing the usual melt quenching procedure. With the use of XRD, the amorphous character of the glasses was confirmed. A high density of 4.530 grams per cubic centimeter is detected in the sample that contains a greater quantity of lead oxide. In order to measure the radiation shielding capabilities of the samples, the Phy-X software was utilized at photon energies ranging from 15 KeV to 15 MeV. Attenuation coefficient is determined to be at its highest for the S1 sample, which has a high density of 270.923 cm-1, according to the findings. The findings indicate that the high-density sample possesses a high level of shielding capabilities against gamma radiation. There is evidence that lead oxide plays a key role in the augmentation of gamma radiation absorption, as demonstrated by the fact that the value of Zeff increased with the amount of PbO present. According to the findings of the data pertaining to the other shielding parameters HVL and MFP, samples that have a high density have a lower value when subjected to high energy. It is concluded that the new glass system that has been developed has the potential to be used for purposes involving the absorption of ionizing radiation.

References

1. Almuqrin, A., Al-Otaibi, J.S., Alwadai, N. *Norah Alwadai, Badriah Albarzan, M. S. Shams, Yasser S. Rammah & R. A. Elsad* Radiation-Shielding, Dielectric, and FTIR Characteristics of Borosilicate Glasses Boosted with Lanthanum Oxide. *J Inorg Organomet Polym* **35**, 10274–10289 (2025). https://doi.org/10.1007/s10904-025-03908-z

2. Sallam, O.I., Kariem, M.A., Abdelrazak, T.A. *Ahmed A. El-Sherif & Eman Yossri Frag.* Determination of Some Optical, Structural and Radiation Shielding Properties of Waste Glass from Cathode Ray Tube. *Silicon* **17**, 3087–3100 (2025). https://doi.org/10.1007/s12633-025-03388-3.
3. Abouhaswa, A.S., Perişanoğlu, U., S. Saltık, N. Ekinci, M. H. Nasr, S. Kalecik & E. Kavaz Perişanoğlu. Er_2O_3-Doped Lead Borate Glasses: Advanced Optical and Radiation Shielding Performance. *J Inorg Organomet Polym* **35**, 4865–4883 (2025). https://doi.org/10.1007/s10904-024-03563-w.
4. J.S. Alzahrani, T. Kavas, R. Kurtulus, I.O. Olarinoye, M.S. Al-Buriahi, Physical, structural, mechanical, and radiation shielding properties of the $PbO–B_2O_3–Bi_2O_3–ZnO$ glass system. J. Mater. Sci. Mater. Electron. **32**, 18994–19009 (2021). https://doi.org/10.1007/s10854-021-06414-3
5. K. Chandra Sekhar, A. Hameed, V.G. Sathe, M. Narasimha Chary, M. Shareefuddin, Physical, optical and structural studies of copper-doped lead oxychloro borate glasses, Bull. Mater. Sci. **41** 79 (2018), https://doi.org/10.1007/s12034-018-1604-
6. Joseph Sumalatha M, Ravi Kumar Guntu, Enhanced photoluminescence and radiation shielding in Mn2+-activated sodium lead borosilicate glasses: Structural and optical insights, Physica B **715** 417612 (2025) https://doi.org/10.1016/j.physb.2025.417612
7. E.A. Abdel Wahab, M.S.I. Koubisy, M.I. Sayyed, K.A. Mahmoud, A.F. Zatsepin, Sayed A. Makhlouf, Kh.S. Shaaban, Novel borosilicate glass system: Na2B4O7-SiO2-MnO2: Synthesis, average electronics polarizability, optical basicity, and gamma-ray shielding features, J Non Cryst Solids **531** 120509 (2021) https://doi.org/10.1016/j.jnoncrysol.2020.120509.
8. K. Chandra Sekhar; N. Narsimlu; G. Nagaraju; J. Laxman Naik; D. Karuna Sagar; Md. Shareefuddin, Radiation shielding features of PbF2-PbO-B2O3-CuO glasses using Phy-X software, AIP Conf. Proc. **3149**, 080012 (2024) https://doi.org/10.1063/5.0224450
9. Erdem Şakar, Özgür Fırat Özpolat, Bünyamin Alım, M.I. Sayyed, Murat Kurudirek, Phy-X / PSD: Development of a user friendly online software for calculation of parameters relevant to radiation shielding and dosimetry, Rad. Phys. Chem. **166** 108496 (2020) https://doi.org/10.1016/j.radphyschem.2019.108496
10. Rabie, G.O., Hammad, A.H. & Abdelghany, A.M. A Comprehensive Evaluation of Structural, Elastic, Optical, and Radiation Shielding Characteristics of Barium Borate Glass Containing Vanadium Ions Using Phy-X/PSD Software and Empirical Approaches. *J. Electron. Mater.* **54**, 5993–6003 (2025). https://doi.org/10.1007/s11664-025-11992-7.
11. G. Nagaraju, Gharam A. Alharshan, K. Chandra Sekhar, Z. A. Alrowaili, Md Shareefuddin, I. O. Olarinoye, D. Karuna Sagar & M. S. Al-Buriah, J Mater Sci: Mater Electron **34**, 374 (2023) https://doi.org/10.1007/s10854-022-09742-0. .
12. Hammam Abdurabu Thabit, Abd Khamim Ismail, S. Hashim, M. I. Sayyed, K. A. Naseer and S. A. Bassam, Designing High-Density of PbO-Enriched Telluro-Borate Glasses for Improved Radiation Shielding: A Comprehensive Study of Attenuation Parameters, ECS J. Solid State Sci. Technol. **12** 113002 (2023) **DOI** 10.1149/2162-8777/ad06e5.
13. Hasan Eskalen, Mustafa Kavgaci, Yusuf Kavun, Hakan Yaykaşli, Harun Gülpak & Mehmet Gök, CuO nanoparticle doping in barium borate glasses: effects on density prediction via machine learning, optical, mechanical, thermal, and radiation protection properties. J Mater Sci: Mater Electron 36, 1135 (2025). https://doi.org/10.1007/s10854-025-15206-y.

14. K Chandra Sekhar, B Srinivas, N Narsimlu, M Narasimha Chary and Md Shareefuddin, The role of halides on a chromium ligand field in lead borate glasses, Mater. Res. Express **4** 105203 (2017), DOI 10.1088/2053-1591/aa8d7e.
15. K. Chandra Sekhar, Abdul Hameed, G. Ramadevudu, M. Narasimha Chary, and Md. Shareefuddin, Physical and spectroscopic studies on manganese ions in lead halo borate glasses, Modern Physics Letters **BVol. 31, No. 16,** 1750180 (2017) https://doi.org/10.1142/S0217984917501809
16. Sukhpal Singh, Ramanpreet Kaur, Saffi Rani, Baltej Singh Sidhu, Investigations on physical, structural and nuclear radiation shielding behaviour of niobium–bismuth–cadmium–zinc borate glass system Progress in Nuclear Energy **142** 104038 (2021) https://doi.org/10.1016/j.pnucene.2021.104038
17. K.A. Mahmoud, O.L. Tashlykov, M.I. Sayyed, Esra Kavaz, The role of cadmium oxides in the enhancement of radiation shielding capacities for alkali borate glasses, Ceramics International **46** 23337–23346 (2020) https://doi.org/10.1016/j.ceramint.2020.02.219
18. Imen Kebaili, Imed Boukhris, M.I. Sayyed, Gamma-ray shielding properties of lead borovanadate glasses, Ceramics International **46** 19624–19628 (2020) https://doi.org/10.1016/j.ceramint.2020.05.032
19. K.C. Sekhar, N. Narsimlu, M.S. Al-Buriahi, H.A. Yakout, I.O. Olarinoye, S. Alomairy, M. Shareefuddin, Synthesis, optical, and radiation attenuation properties of CaF_2–TeO_2–$Na_2B_4O_7$–CuO glass system for advanced shielding applications. Eur. Phys. J. Plus. **136**, 903 (2021). https://doi.org/10.1140/epjp/s13360-021-01906-x
20. K Chandra Sekhar, Md Shareefuddin, A El-Denglawey and Yasser B Saddeek, Phys. Scr. 97 035704 (2022), https://doi.org/10.1088/1402-4896/ac53c7
21. Rajesham Siddoju, Chandrasekhar M., Chandra Sekhar K., Shankar J., J. Anjaiah and Siva Kumar J., Impact on Structural and Radiation Shielding Features of 60B2O3-20CdO-5Al2O3-(15-x) CaF2-xMoO3, ECS J. Solid State Sci. Technol. **14** 056004 (2025) **DOI** 10.1149/2162-8777/add377.
22. Hassan Hanafy, K. ChandraSekhar, Reda Elsaman, K.A. Aly, Nissamudeen, M. Alhab radi, G. Nagaraju, Mohd Shakir Khan, Yasser B. Saddeek, Probing the synergistic impacts of different lead halides in MoO3-Borobismuthate glass systems for improved radiation-blocking and rigidity features, Nuclear Instruments and Methods in Physics Research Section B: **563** 165708 (2025) https://doi.org/10.1016/j.nimb.2025.165708