



# Biyoaktif Camların Etkin Atom Numaraları ve Kütle Azaltma Katsayıları Üzerine Bir Araştırma

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## Özet

Biyoaktif bir malzeme, vücuttan dokuya bağlanma gibi belirli bir biyolojik yanıt sağlayan doğal veya insan yapımı bir materyal olarak bilinir. Hastalıklı ve hasarlı dokuların onarımı ve rekonstrüksiyonunda ve doku ve sert doku (kemik) yeniden yapılanmasında sayısız uygulamaları vardır. Bu çalışmada, seçilen biyoaktif camlar için kütle azaltma katsayısı ( $\mu / \rho$ ), etkin atom numarası ( $Z_{\text{eff}}$ ), yarı değer kalınlığı (HVL) ve ortalama serbest yol (MFP) gibi gama ışını zırlama parametrelerini değerlendirdik. Seçilen camların zırlama etkileri birbirleriyle karşılaştırılabilir. Etkin atom numarası ( $Z_{\text{eff}}$ ), çok elementli bir malzemenin teknik ve endüstriyel uygulamalarını, radyasyon tepkisini, radyasyon zırlama tasarımını, emilen dozun miktarını tespit etmek için kullanılan uygun bir parametredir. Bu nedenle, bu parametreyi kesin olarak belirlemek için doğru yöntemi seçmek çok önemlidir. Bu çalışmada, 1 keV ile 100 GeV enerji bölgesinde toplam foton etkileşimi için hesaplama yöntemi kullanılarak farklı tipte malzemelerin etkili atom numarası hesaplanmıştır. Bu çalışmadan elde edilen sonuçlar, etkin atom numarasının, düşük ve daha yüksek enerji bölgesindeki etkileşimli malzemenin kimyasal bileşimine güçlü bir şekilde bağlı olduğunu, ancak orta enerji bölgesinde, kimyasal bileşim bağımlılığının çok zayıfladığını göstermektedir. Bu sonuç, biyoaktif camların bileşiminde  $P_2O_5$  içeriğindeki bir artışın malzemelerin biyoaktivitesinin artmasıyla sonuçlandığı şeklinde yorumlanabilir. Bu nedenle, bu çalışma biyoaktif camların biyomedikal uygulamalar için potansiyel biyomalzemeler olacağını ortaya koymaktadır.

**Anahtar Kelimeler:** Biyoaktif Camlar, Kütle Azaltma Katsayısı, Etkin Atom Numarası, Radyasyon Zırlama

## An Investigation on Effective Atomic Numbers and Mass Attenuation Coefficients of Some Bioactive Glasses

### Abstract

A bioactive material is known as a natural or man-made material that prompts a specific biological response from the body such as bonding to tissue. They have numerous applications in the repair and reconstruction of diseased and damaged tissue, and tissue and hard tissue (bone) re-engineering. In this study, we have evaluated the same gamma-ray shielding parameters such as mass attenuation coefficient ( $\mu/\rho$ ), effective atomic number ( $Z_{\text{eff}}$ ), half value layer (HVL), mean free path (MFP) for selected bioactive glasses. The shielding effectiveness of the selected glasses is found comparable each other. Effective atomic number ( $Z_{\text{eff}}$ ) is convenient parameters used to characterize the radiation response of a multi-element material in the technical and industrial applications, radiation shielding design, absorbed dose. Thus, it is very significant to choose accurate method to determine this parameter unambiguously. In the present study, effective atomic number of different type of material has been calculated by using calculation method for total photon interaction in the energy region of 1 keV to 100 GeV. The results obtained from this study show that effective atomic number depends strongly on the chemical composition of the interaction material in the lower as well as higher energy region, but in the intermediate energy region, the chemical composition dependence becomes very weak. This result can be interpreted that an increase in  $P_2O_5$  content in the composition of bioactive glasses results as an increase of bioactivity of that particular materials. Therefore, this study underlines the finding that bioactive glasses would be potential biomaterials for biomedical applications.

**Keywords:** Bioactive Glasses, Mass Attenuation Coefficient, Effective Atomic Number, Radiation Shielding

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## 1. Introduction

Radiation interaction with matter has become a considerable subject with the extensive use of X-ray and/or gamma-ray in various fields such as reactors, nuclear power plants, nuclear engineering, space technology, nuclear diagnostics, nuclear medicine, radiation dosimetry and radiation biophysics, technological and engineering applications. Due to the increasing usage of the radiation, the term of risk on human health should be considered. Therefore, the use of shielding materials is very important in the mentioned fields. To choose an appropriate type of material, radiation interaction parameters such as mass attenuation coefficient, effective atomic number should be determined. The mass attenuation coefficients (MAC) measures the likelihood of interaction that happens between photons and matter of unit mass per unit area. The MAC for natural and other critical materials is important for modern, organic, horticultural and restorative applications (Jackson & Hawkes, 1981). An accurate estimation for MAC has to be made beforehand to determine the basic information in number of fields, for example, atomic diagnostics, radiation security, atomic medication, radiation dosimetry, gamma beam, radiation biophysics and so forth. In addition, the mass attenuation coefficients are generally utilized in the calculation of photon penetration and energy deposition in organic, shielding and other dosimetric materials. Hine has brought up that in composite materials, for photon interactions, a solitary number can't speak for the exact atomic number across different energy regions (Hine, 1952). This number for composite materials is called as "effective atomic number ( $Z_{\text{eff}}$ )" and it varies with photon energy. The energy absorption in a given medium can be determined if certain constants are known. Therefore, the investigation of effective atomic number is exceptionally helpful for some innovative applications. The effective atomic number is likewise helpful in medicinal radiation dosimetry for the estimation of dose in radiation treatment and therapeutic medical imaging.

Practical application of certain material for radiation attenuation depends on parameters like mass attenuation coefficient ( $\mu/\rho$ ), effective atomic number ( $Z_{\text{eff}}$ ), mean free path (MFP), and half value layer (HVL). These parameters are used to determine the scattering and absorption of gamma-rays both theoretically, empirically and practically. The best radiation attenuation derives from photon energy, material density and an atomic number of elements present in the materials. In the present study, MAC,  $Z_{\text{eff}}$ , MFP and HVL values are calculated for three bioactive glasses that are listed as follows: H, HP5, HP6.5 against photon energies of 0.02 MeV, 0.06 MeV, 0.08 MeV, 0.122 MeV, 0.356 MeV, 0.511 MeV, 0.662 MeV, 1.173 MeV, 1.25 MeV, 1.33 MeV, 5 MeV, 8 MeV, 10 MeV, 15 MeV and 20 MeV.

## 2. Materials ve Method

### 2.1. Selected Bioactive Glasses

A bioactive material is known as a natural or man-made material that prompts a specific biological response from the body such as bonding to tissue. They have numerous applications in the repair and reconstruction of diseased and damaged tissue, and tissue and hard tissue (bone) re-engineering. Bioactive glasses are one type of biomaterials along with polymers, metals, composites, and ceramics. They are closely related to bio ceramics, yet they have an important advantage over other types of bioactive ceramics by enabling to control a range of chemical properties and rate of binding to tissue. Bioactive glasses were first found by Hench et.(Hench & Andersson, 1993). Al around 1960s as such compositions and crystallized ceramics in the  $\text{Na}_2\text{O}-\text{CaO}-\text{P}_2\text{O}_5-\text{SiO}_2$  system, which is the base components of bioactive glasses, provides strong bonds with living tissues (Kaur et al., 2014). The conventional glass manufacturing is also applied to the production of bioactive glasses and the invention of bioactivity was a revolutionary practice in tissue implants. In the manufacturing and design processes, one of the important issues is that they should provide appropriate structural compatibility without any detrimental effects on living tissues. In this sense, there is a reverse linkage between the degree of crystallization and bioactivity, as the crystallization and the structural strength increase bioactivity is greatly reduced.

However, bioactive glasses with high structural strength can also be used for radiation shielding purposes. Glasses used for radiation shielding should have high interaction cross-section. This investigation deals with bioactive glasses consisting of the different percentage of  $\text{Na}_2\text{O}-\text{CaO}-\text{P}_2\text{O}_5-\text{SiO}_2$  in the composite. Table 1 shows the chemical compositions of investigation bioactive glasses(Doweidar, 2009).

Table 1: Chemical names and formulas for the bioactive glasses

	SiO <sub>2</sub> (mol%)	Na <sub>2</sub> O (mol%)	CaO (mol%)	P <sub>2</sub> O <sub>5</sub> (mol%)	D <sub>c</sub> (g/cm <sup>3</sup> )
H	46.20	24.30	26.90	2.60	2.729
HP5	43.70	24.40	26.90	5.00	2.720
HP6.5	42.20	24.30	26.90	6.50	2.714

## 2.2. Method

### 2.2.1 Mass Attenuation Coefficient (MAC)

MAC values for gamma rays are one of the most useful parameters for radiation shielding along with many other applications such as nuclear research centers, radiations etc. The number of photons interacted with the medium is measured by the MAC. The MAC values of the compound using the mixture rule given by the following equation:

$$\mu/\rho = \sum_i w_i(\mu/\rho)_i$$

where  $w_i$  denotes the fractional weight of the  $i$ th constituent in the elements, The MAC value at certain energy of any element is calculated by using Xcom software.

### 2.2.2 The Linear Attenuation Coefficient (LAC)

LAC (in  $\text{cm}^{-1}$ ) is multiplication of MAC value and density of the compound. The linear attenuation coefficient for a material depends on the incident photon energy, atomic number and density. For the selected samples, MAC are calculated using the mixture rule as given below;

$$LAC = \left(\frac{\mu}{\rho}\right)\rho$$

where  $w_i$  is the proportion by weight and  $(\mu/\rho)_i$  is the mass attenuation coefficient of the  $i$ th element. The  $(\mu/\rho)_i$  values can be calculated by using Xcom software.

### 2.2.3 Half Value Layer (HVL)

HVL is one of the appropriate parameter denoting gamma ray interaction of a material. HVL is used to signify the particular thickness of the material that is required to decrease intensity of the photon %50 of its initial value. In this case, HVL characterizes the effectiveness of gamma ray shielding (Dong, El-Mallawany, Sayyed, & Tekin, 2017). The following equation is used to calculate the HVL

$$HVL = \frac{0.693}{\mu}$$

Where  $\mu$  ( $\text{cm}^{-1}$ ) is linear attenuation coefficient is determined by the multiplication of the mass attenuation coefficient value ( $\mu$ ) and density of the sample ( $\rho$ ).

### 2.2.4 Tenth-value Layer (TVL)

To reduce the intensity of gamma-ray, the thickness of the concrete shielding material has to be adjusted. Reducing the intensity of the gamma-ray to  $1/10^{\text{th}}$  is called TVL, tenth-value layer, which is calculated by using the following formula

$$TVL = \frac{2.303}{\mu}$$

where  $\mu$  is linear attenuation coefficient.

Both HVL and TVL is very useful for approximate shielding calculations. Once HVL and TVL values are calculated, the penetration of the gamma ray through all variants of thicknesses and density of sample can be easily determined.

### 2.2.5 Mean Free Path (MFP)

MFP is another important parameter denoting gamma ray interaction of a material. Before an interaction occurs, a photon in the medium travels for while and MFP represents the distance traveled by a moving photon between sequential collisions.

$$MFP = \frac{1}{\mu}$$

where  $\mu$  ( $\text{cm}^{-1}$ ) is again linear attenuation coefficient that is equal to multiplication of the mass attenuation coefficient value and density of the sample. The mean free path is also reciprocal of linear attenuation coefficient.

### 2.2.6 Effective Atomic Number ( $Z_{\text{eff}}$ )

$Z_{\text{eff}}$  is a fitting quantity for corresponding gamma ray interactions.  $Z_{\text{eff}}$  is a parameter similar to the atomic number of elements, which describes the properties of the composite materials (compounds or mixtures) in terms of equivalent elements, and it varies with energy (Sayyed, 2016). That is,  $Z_{\text{eff}}$  changes with photon energy for composite materials on the contrary to single number cannot. It can also be derived by the following formula

$$Z_{\text{eff}} = \frac{\sigma_a}{\sigma_e}$$

Where  $\sigma_a$  and  $\sigma_e$  which can be calculated by the formula below, are correspondingly the total atomic cross section and total electronic cross section:

$$\sigma_a = \frac{\mu/\rho}{N_A \sum_i \frac{w_i}{A_i}}$$

$$\sigma_e = \frac{1}{N_A} \sum_i \left( \sum_j \frac{f_j A_j}{A_j} \right) w_i$$

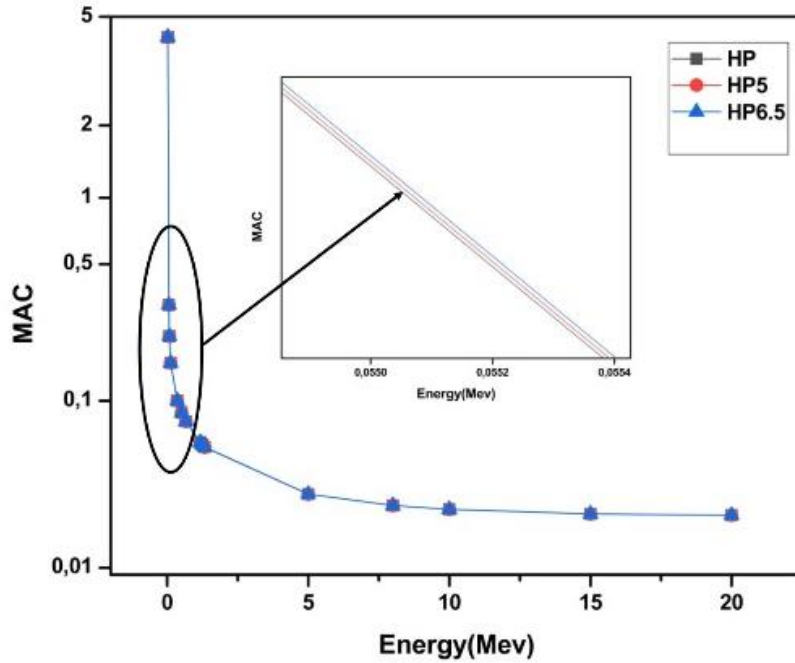
Where  $A_i, Z_i, f_i$  are respectively the atomic number and fractional abundance of element  $i$ ,  $N_A$  corresponds Avogadro constant.

### 2.2.7 Xcom

Xcom is a software that generates total cross sections, attenuation coefficients as well as partial cross sections for various interaction processes such as incoherent and coherent scattering, photoelectric absorption and pair production, for elements, compounds and mixtures as needed at energies from 1 keV to 100 GeV. Xcom software, in which material types were defined by their elemental fractions, is a user-friendly calculation program and input parameter specifications are quite understandable and easy to access (M. Berger, 2010; M. J. Berger, 1998).

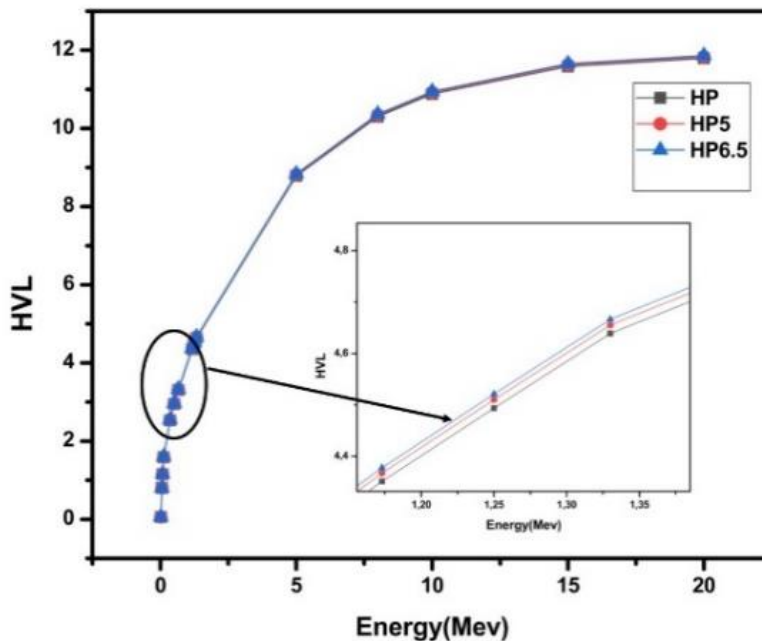
## 3. Result and Discussion

In the present study, mass attenuation coefficients ( $\mu/\rho$ ) of three bioactive glasses namely H, HP5, HP6.5 are examined by using the XCOM program based on the mixture rule at photon energies of 0.02 MeV, 0.06 MeV, 0.08 MeV, 0.122 MeV, 0.356 MeV, 0.511 MeV, 0.662 MeV, 1.173 MeV, 1.25 MeV, 1.33 MeV, 5 MeV, 8 MeV, 10 MeV, 15 MeV and 20 MeV. The mass attenuation coefficients ( $\mu/\rho$ ) has been presented in the Fig.1. According to Fig.1, the  $\mu/\rho$  for all samples decreases with increasing the photon energy from 0.02 MeV to 20 MeV. This can be interpreted that the interaction occurs between the photons and the bioactive glasses in the low energy region whereas in the high energy region interaction is decreasing. Thus, as the photon energy increases, more photons infiltrate into the bioactive glasses. From the Fig.1, which shows the variation in the  $\mu/\rho$  value with the photon energy for bioactive glasses studied in this work, it very well may be seen that the  $\mu/\rho$  values rely upon the photon energy notwithstanding the chemical composition of the glasses. The variation of  $\mu/\rho$  with the photon energy for all the selected glasses is almost equivalent to each other. While the values of  $\mu/\rho$  for these glasses in the low-energy area are higher in magnitude, they decline rapidly with expanding the energy. (S. A. Issa et al., 2019)



*Figure 1: MAC for Bioactive glasses*

This bioactive glasses comprising of the distinctive level of  $\text{Na}_2\text{O}-\text{CaO}-\text{P}_2\text{O}_5-\text{SiO}_2$  in the composite. Obviously the  $\mu/\rho$  for all the examined glasses diminishes with the increment of photon energy up to 5 MeV. Thereafter, the the value of  $\mu/\rho$  turns out to be almost constant in the high energy region. Meanwhile, it is observed that the maximum value for  $\mu/\rho$  was found for HP6.5 glasses. This result derives from the fact that these glasses contain high  $\text{P}_2\text{O}_5$  and low  $\text{SiO}_2$  in their composition. As the rate of  $\text{P}_2\text{O}_5$  admixture increase and  $\text{SiO}_2$  decrease, the shielding properties for these selected bioactive glasses vary. The best shielding properties, therefore, has been seen from HP6.5. Therefore, one can infer that variety of  $\mu/\rho$  relies upon first and foremost the composition of the glass system, which is lower for a low-Z element and vice versa in the prepared glasses. At whatever point we find the lower estimation of MFP, that gives us a tangible indication for the interaction of radiation with the medium and consequently the ideal shielding properties are accomplished (Tekin, Altunsoy, Ozturk, Kilicoglu, & Sayyed, 2018; Tekin, Erguzel, et al., 2018).



*Figure 2: HVL for Bioactive glasses*

The HVL variation in photon energy range 1 keV to 100 GeV is depicted in the Fig.2, which shows also that in the low energy range ( $E < 0.08$  MeV) the HVL values for the glasses are very small. The HVL begins increasing once the photon energy cross this low energy range and shows its highest rate at about 10 MeV. Thereafter, it starts decreasing becomes almost constant at 20 MeV photon energy. HP glasses are the one with minimum HVL values, and HP6.5 is the highest HVL from which we can arrive the conclusion that the HP have superior shielding capability against gamma radiation. The variation of HVL with the photon energy for the present bioactive glasses are shown graphically in the Fig.2. The HVL is seen to rise as the energy of the photon increases. It should be underlined that H and HP5 having smaller HVL values comparing with rest of bioactive glasses because they have higher density (and it is well known that the HVL depends inversely on the density of the samples).

On the other hand, the mean free path (MFP) of a certain material is the average distance traveled by a moving photon between sequential collisions. The MFP ( $1/\mu$ ) for the 3 bioactive glasses are calculated in the energy range of 0.02–20 MeV. MFP values for H, HP5, HP6.5 are in the range of 0.086159- 17.019721 cm, 0.086343- 17.076036 cm, 0.086392- 17.113787 cm respectively. The mean free path (MFP) is the average distance traveled by a moving particle (such as an atom, a molecule, a photon) between successive impacts (collisions). From Fig.3, it is clear that, the values of MFP increase with the photon energy increasement. In the photon energy range 0,02-0,08 MeV, the values of mean free path are very small. Also, the values of MFP increase rapidly in this energy range. In the photon energy range 0.122-5 MeV the values of MFP of all samples increase slower than increase in the lower photon energy range. In the higher photon energy ( $E > 5$  MeV), the values of mean free path are independent on photon energy.

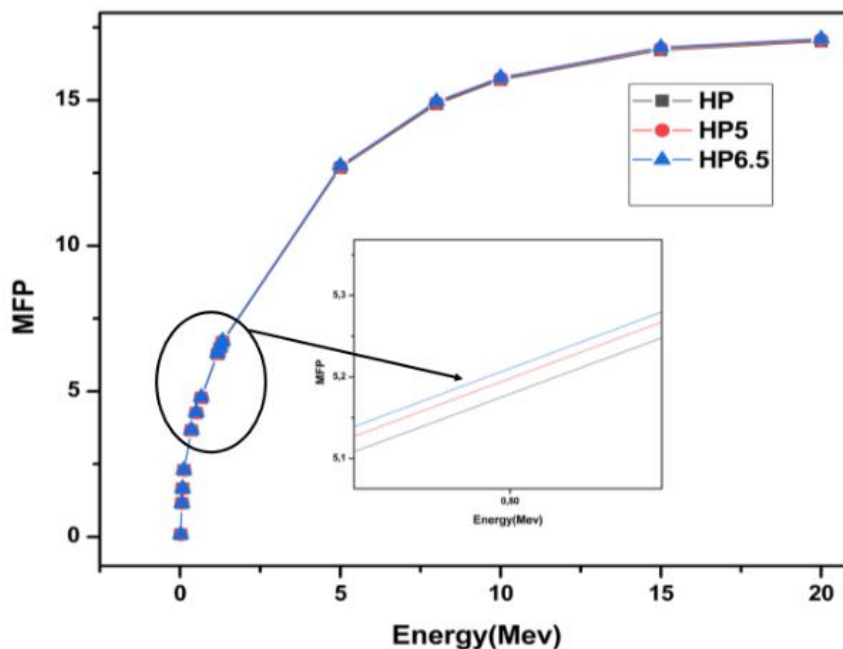


Figure 3: MFP for Bioactive glasses

The effective atomic number,  $Z_{\text{eff}}$ , reveals the energy-dependent behavior of the compounds. The calculated  $Z_{\text{eff}}$  for these bioactive glasses are reviewed in the graph. It is observed that the  $Z_{\text{eff}}$  values for the 3 bioactive glasses are nearly constant in the energy region between 0.02 and 20 MeV due to incoherent (Compton) scattering.

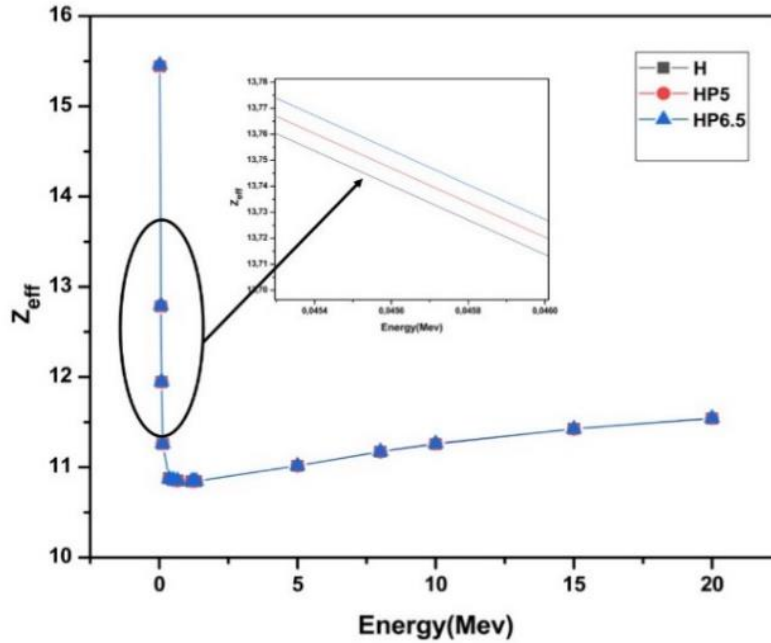


Figure 4:  $Z_{eff}$  for Bioactive glasses

From the graph above, it can be seen that HP5 and HP6.5 having the highest  $Z_{eff}$  values among investigated bioactive glasses on the following ranges 15.448- 11.543 MeV and 15.459- 11.546 MeV respectively. Effective atomic numbers of 3 bioactive glasses for total photon interactions in the wide energy range of 0.02 MeV to 20 MeV. Moreover, the graph shows that the  $Z_{eff}$  values for the selected bioactive glasses diverge between 15.459 MeV and 11.539MeV. All the 3 bioactive glasses consist of Si, Na, Ca, P and O. Therefore, the  $Z_{eff}$  values for the 3 bioactive glasses molecules lie in between the atomic number of these elements. Effective atomic numbers,  $Z_{eff}$ , of the bioactive glasses are shown in the Fig.4. The variation of  $Z_{eff}$  with associated photon energy for these compounds are given in the Fig.4, which shows that  $Z_{eff}$  is a function of photon energy. (Sayyed, Issa, Tekin, & Saddeek, 2018) Briefly, variation in  $Z_{eff}$  can be classified into three energy regions- low-intermediate-and high- and all these regions occurs due different photon interactions. At low energy region, photoelectric absorption is the dominating photon interaction process. In the Fig.4, below 0.122 MeV, photoelectric process is dominant and thus, the variation of  $Z_{eff}$  is large. At the intermediate energy region, the dominant process is Compton scattering. In the Fig.4, between 0.356 MeV < E < 1.33 MeV the variation is almost constant because the Compton scattering process. At the high energy region, the dominating process is pair production. In the Fig.4, between 5 to 20 MeV, pair production process becomes dominant. In this sense, all variations are to be explained by Z dependence of total atomic cross sections and the photoelectric absorption cross-section gives higher weight to the high Z elements than the other processes. However, the Compton scattering cross-section is proportional to Z, giving less weight to the high Z elements than photon electric absorption and pair production processes. All in all, in the low-energy range (E< 0.356 MeV) where  $Z^4$  dependence of the photoelectric absorption cross section gives a heavy weight for the highest atomic number of the compound,  $Z_{eff}$  reaches its maximum value. At high energies, typically above 5 MeV,  $Z_{eff}$  is again constant but smaller than in the low-energy range. This is due to the dominance of pair production, the cross section of which has a weaker  $Z^2$  dependence.(S. A. M. Issa, Saddeek, Sayyed, Tekin, & Kilicoglu, 2019; Sayyed, Tekin, Kılıcoglu, Agar, & Zaid, 2018; Tekin, Sayyed, et al., 2018)

### 3. Conclusion

In this work, mass attenuation coefficient (MAC), mean free path (MFP), half value layer (HVL) and effective atomic number ( $Z_{eff}$ ) has been calculated for selected bioactive glasses by using a direct method for total photon interaction in the energy region from 1 keV- 100 GeV using Xcom program. The results obtained from this study show that effective atomic number depends strongly on the chemical composition of the interaction material in the lower as well as higher energy region, but in the intermediate energy region, the chemical composition dependence becomes very weak. This result can be interpreted that an increase in  $P_2O_5$  content in the composition of bioactive glasses results as an increase of bioactivity of that particular materials. Therefore, this study underlines the finding that bioactive glasses would be potential biomaterials for biomedical applications.

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