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Investigation of photon energy absorption properties for some biomolecules

Mohammed Sultan Al-Buriahi[1] · Halil Arslan[2] · Baris T. Tonguc[1]

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Abstract The mass energy absorption coefficient (μ_{en}/ρ), effective atomic number ($Z_{PEA_{eff}}$), and electron density ($N_{PEA_{eff}}$) of some biomolecules with potential application in radiation dosimetry were calculated for their photon energy absorption (PEA) in the energy region of 1–20 MeV. It was noticed that the values of μ_{en}/ρ, $Z_{PEA_{eff}}$, and $N_{PEA_{eff}}$ vary with the energy and composition of the biomolecules. The results for $Z_{PEA_{eff}}$ were compared with effective atomic numbers ($Z_{PI_{eff}}$) owing to the photon interaction (PI). Significant differences were noted between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ in the energy region of 10–150 keV for all of the biomolecules involved. A maximum difference of 45.36% was observed at 50 keV for creatinine hydrochloride. Moreover, the studied attenuation parameters were found to be sharply affected at the K-absorption edge of relatively high-Z elements present in the biomolecules.

Keywords Photon energy absorption · Effective atomic number · Electron density · Biomolecule

1 Introduction

There is considerable interest in radiation dosimetry resulting from photon interaction and photon energy absorption, especially in medical applications such as radiology and radiation protection. The method in which photons are dissipated in a medium is complicated, and the nature of the mechanism that may occur depends on the photon energy and atomic number of the material. The atomic number for a complex medium (e.g., a biomolecule) is not constant but varies with the photon energy and called the effective atomic number [1]. In fact, there are two types of effective atomic number: the effective atomic number for photon interaction and the effective atomic number for photon energy absorption. $Z_{PI_{eff}}$ is more common because it can be obtained experimentally by using the transmission geometry from the mass attenuation coefficient (μ/ρ), which is a convenient parameter for representing the photon interaction. Similarly, $Z_{PEA_{eff}}$ is more useful for dose calculation [2], and it can be obtained from the energy absorption coefficient (μ_{en}/ρ), which is a convenient parameter for representing the photon energy absorption in a complex medium [3–6]. The parameters of μ/ρ and μ_{en}/ρ are comprehensively discussed in the first two chapters of a book edited by Hine and Brownell [7]. In this book, the mass attenuation coefficient was referred to as the total absorption coefficient and the mass energy absorption coefficient as the true absorption coefficient. These coefficients are related by the equation [$\mu/\rho = \mu_{en}/\rho + \mu_s/\rho$], where μ_s/ρ is the scatter absorption coefficient. Briefly, μ/ρ is a measure of the probability of collision between the photon and material in units of mass per unit area. By contrast, μ_{en}/ρ is a measure of the average fractional amount of incident photon energy transferred to the kinetic energy of charged particles as a result of these interactions [8]. These basic quantities, which have been widely used as a reference database, were provided in numerous tabulations and software [9–13].

Knowledge of photon energy absorption parameters such as μ_{en}/ρ, $Z_{PEA_{eff}}$, and $N_{PEA_{eff}}$ for biomolecules is

✉ Mohammed Sultan Al-Buriahi
mburiahi@gstd.sci.cu.edu.eg

[1] Department of Physics, Sakarya University, Sakarya, Turkey

[2] Electrical and Electronics Engineering, Sakarya University of Applied Sciences, Sakarya, Turkey

important when estimating the radiation biological effect from a dose that is received by biomolecules, which are the main components in tissues [2]. The biomolecule is an organic compound that governs a variety of activities in living organisms. Living systems are made up of various complex biomolecules such as carbohydrates, proteins, nucleic acids, and fats. In particular, proteins catalyze reactions, transport oxygen, and perform other important tasks. For example, creatinine hydrochloride is used for investigations of drug distribution in the body. More knowledge about the importance and applications of selected biomolecules can be found elsewhere [8, 14]. Moreover, photon attenuation parameters for the biomolecules are required in radiography and radiation therapy, where the cross-sectional anatomy is obtained by computer-assisted tomography (CAT) scans [15]. Over the past 15 years, many authors published extensive research based on $Z_{PI_{eff}}$ calculations for different materials using different methods [16–29]. Awasarmol et al. [18] studied some organic materials used for radiation dosimetry by using an experimental transmission method in the energy range of 122–1330 keV. Elbashir et al. [20] compared the experimental values of $Z_{PI_{eff}}$ with Monte Carlo simulation results by using MCNP5 for six samples of amino acids in the energy range of 0.122–1.330 MeV. Kurudirek et al. [26] calculated $Z_{PI_{eff}}$ and $N_{PI_{eff}}$ for essential biomolecules over a wide range of energies from 10 keV to 1 GeV. However, such studies, chiefly for biomolecules, for $Z_{PEA_{eff}}$ appear to be scarce [30–33]. Hubbell1977 [30] presented the first study of photon mass attenuation and mass energy absorption coefficients for H, C, N, O, Ar, and seven mixtures from 0.1 keV to 20 MeV. Later, Singh et al. [33] succeeded for the first time in determining the mass energy absorption coefficient by using Geant4 simulations. Very recently, numerous experiments were performed to determine μ/ρ and $Z_{PI_{eff}}$ for some biological compounds at photon energies of 81, 122, 356, 511, 662, 1170, 1275, and 1332 keV [34–37] with significant success. The energy absorption parameters for these biomolecules have not yet been mentioned in the literature, and this is the main goal of the present work.

In the present work, photon energy absorption parameters (μ_{en}/ρ, $Z_{PEA_{eff}}$, and $N_{PEA_{eff}}$) for the biomolecules given in Table 1 are calculated in the energy region of 1 keV–20 MeV. The interpolation method is applied to extract the values of μ_{en}/ρ at the absorption edges of the biomolecule constituents. The ratios of $Z_{PEA_{eff}}$ for the biomolecules to that for water ($Z_{RW_{eff}}$) are also reported. The results for $Z_{PEA_{eff}}$ are compared with the values of $Z_{PI_{eff}}$, which were investigated in our previous work [38]. Moreover, atypical changes in the photon energy absorption properties obtained at the K-absorption edge of relatively high-Z elements present in biomolecules are discussed.

Table 1 Chemical formula and mean atomic number of studied biomolecules

Name	Formula	$\langle Z \rangle$
Creatinine H	$C_4H_8ClN_3O$	4.59
Glycoprotein	$C_{28}H_{47}N_5O_{18}$	4.02
Glycine	$C_2H_5NO_2$	4.00
Lactose	$C_{12}H_{22}O_{11}$	4.04
Margaric acid	$C_{17}H_{34}O_2$	2.87
Tyrosine	$C_6H_{11}NO_3$	3.71
Inosine	$C_{10}H_{12}N_4O_5$	4.52
Proline	$C_5H_9NO_2$	3.65

2 Methods of calculation

$Z_{PEA_{eff}}$ can be calculated by using the values of μ_{en}/ρ, which are obtained by the additivity rule [39]. For a type of biomolecule, the mass energy absorption coefficient is calculated by

$$(\mu_{en}/\rho)_{bio} = \sum_i w_i (\mu_{en}/\rho)_i, \tag{1}$$

where w_i and μ_{en}/ρ are the weight fraction and the mass energy absorption coefficient of the ith constituent element in the biomolecule, respectively. The μ_{en}/ρ values of the constituent elements of the biomolecules are taken from a compilation by Hubbell and Seltzer [9]. Then, $Z_{PEA_{eff}}$ is given by

$$Z_{PEA_{eff}} = \frac{\sum_i f_i A_i (\mu_{en}/\rho)_i}{\sum_j \frac{f_j A_j}{Z_j} (\mu_{en}/\rho)_j}, \tag{2}$$

where Z_i is the atomic number, A_i is the atomic weight, and f_i is the fractional abundance of each constituent element provided that $\sum_i f_i = 1$. $Z_{PI_{eff}}$ can be obtained from Eq. 2 by substituting the mass attenuation coefficient for the mass energy absorption coefficient [40, 41]. The effective electron density is taken into account to determine the likelihood of the Compton effect and is expressed by the relation of

$$N_{PEA_{eff}} = N_A \frac{n Z_{PEA_{eff}}}{\sum_i n_i A_i} \quad \text{(electrons/g)}, \tag{3}$$

where N_A is Avogadro's number and n is the total number of atoms in the biomolecule[42].

The mean atomic number $\langle Z \rangle$ is derived from a chemical formula such as $\langle Z \rangle = \sum_i n_i Z_i / n$. Furthermore, another parameter, the effective atomic number relative to

water ($Z_{RW_{eff}}$), is the ratio between the $Z_{PEA_{eff}}$ values of the biomolecule and of water.

$$Z_{RW_{eff}} = \frac{(Z_{PEA_{eff}})_{bio}}{(Z_{PEA_{eff}})_{water}}. \quad (4)$$

For this equation, $Z_{PEA_{eff}}$ of water is obtained by using the same method that is utilized for the studied biomolecules.

Finally, we use an interpolation method to find μ_{en}/ρ values of the elements in creatinine hydrochloride at the Cl K-edge (2.47 keV). This method is described in our previous work [38]. Briefly, for each of the elements in creatinine hydrochloride, the plot of μ_{en}/ρ vs. the photon energy is a smooth continuous function. Then, by matching a selected energy with the corresponding value of μ_{en}/ρ, we find the value of μ_{en}/ρ at 2.47 keV.

3 Results and discussion

The variations of the mass energy absorption coefficient with photon energy for biomolecules are shown in Fig. 1. It can be seen that μ_{en}/ρ depends not only on the chemical compositions of the biomolecules but also on the photon energy. The energy dependence of μ_{en}/ρ can be analyzed by dividing the photon energies into three regions.

In the first region, the photon energy is slightly higher than the binding energy of the electrons in their atoms. Here, the photoelectric effect is the predominant process and may cause a sharp change in the attenuation properties owing to the existence of high-Z elements in the sample. As seen in the case of creatinine hydrochloride, there are two values for μ_{en}/ρ at 2.82 keV owing to the chloride K-absorption edge: the upper side with a value of 1.5×10^2 cm^2/g and the lower side with a value of 4.9×10^2 cm^2/g. It should be mentioned that the μ_{en}/ρ values of all constituent elements of creatinine

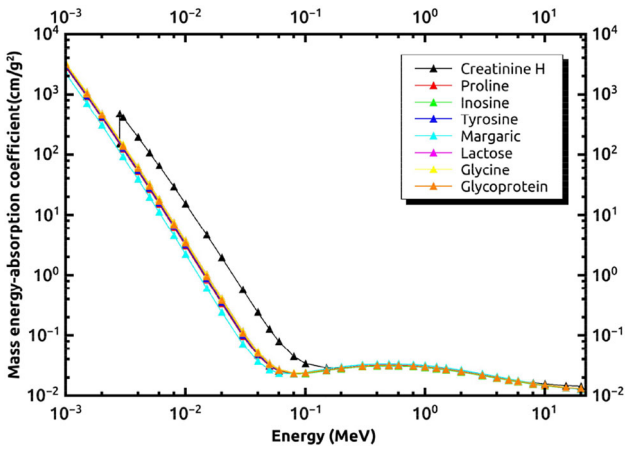

Fig. 1 Mass energy absorption coefficient (μ_{en}/ρ) as a function of photon energy for biomolecules

hydrochloride are not available in the compilation by Hubbell and Seltzer [9] at 2.82 keV, so the interpolation method is adopted to find the μ_{en}/ρ values of all constituent elements of creatinine hydrochloride at the K-absorption edge of Cl [38, 42]. It is worth mentioning that all samples except for creatinine hydrochloride consist of low-Z elements. Therefore, the K-absorption edge is not observed because the K-shell binding energy for the low-Z elements is on the order of few hundred electron volts (e.g., it is 543.1 eV for oxygen). Thus, the K-absorption edges do exist but are not detectable, e.g., the weak photons (in the eV range) survive for about 1 μ, and then they are absorbed.

The second region exhibits Compton scattering as the main contributor to the attenuation process. The attenuation, in this case, is independent of the effective atomic number and dependent on the electron density. When increasing the photon energy to 1.022 MeV, the third region represented by the pair production becomes the dominant process of the attenuation. These processes will be more apparent in the discussion of the variation of the effective atomic number with the photon energy.

The calculation results for $Z_{PEA_{eff}}$ with $Z_{PI_{eff}}$ values at various photon energies are given in Tables 2 and 3. In addition, from Figs. 2, 3, 4 and 5, it can be seen that the variation of $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ with the energy is approximately similar for all of the biomolecules studied except for abrupt changes (e.g., two values of the attenuation at the same energy) near the K-absorption edge of Cl in creatinine hydrochloride.

The $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ values for creatinine hydrochloride regularly increase to 4 to 15 keV and then regularly decrease to 200–600 keV (see Fig. 2). After that, these values remain almost constant up to 1.5–2 MeV. From 2.0 MeV, they increase with the photon energy to 20 MeV. By comparing Z_{PAeff}, $Z_{PI_{eff}}$, and $Z_{RW_{eff}}$, we noticed that $Z_{RW_{eff}}$ does not show strong energy dependence. For example, it takes values between 1 and 3 for all of the biomolecules studied along the considered photon energy range. This parameter is a rough estimate to mimic the scan in the patient. Furthermore, $\langle Z \rangle$ is equal to the effective atomic numbers over a wide energy range around 1 MeV where Compton scattering is the main process.

The variation of $Z_{PEA_{eff}}$ is attributed to the relative domination of partial photon attenuation. In fact, there is a unique effective atomic number for each attenuation process. For example, for the attenuation values that come from photoelectric absorption, one can obtain the effective atomic number of the photoelectric absorption and so on for other attenuation processes. In this work, the total effective atomic number (for all attenuation processes) is investigated. At low energies, the photoelectric effect is

Table 2 Effective atomic numbers for photon energy absorption and photon interaction for creatinine hydrochloride, glycoprotein, glycine, and lactose

E (MeV)	Creatinine H		Glycoprotein		Glycine		Lactose	
	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$
1.00E−03	7.952	7.952	7.122	7.121	7.274	7.274	7.304	7.303
1.50E−03	8.029	8.030	7.150	7.151	7.298	7.299	7.333	7.334
2.00E−03	8.094	8.094	7.166	7.168	7.310	7.313	7.349	7.351
3.00E−03	12.952	12.783	7.181	7.189	7.321	7.330	7.364	7.373
4.00E−03	13.239	13.142	7.181	7.202	7.320	7.340	7.364	7.385
5.00E−03	13.423	13.385	7.170	7.210	7.307	7.347	7.354	7.393
6.00E−03	13.542	13.565	7.148	7.217	7.284	7.353	7.332	7.400
8.00E−03	13.643	13.806	7.066	7.226	7.200	7.359	7.251	7.409
1.00E−02	13.611	13.969	6.930	7.230	7.062	7.362	7.115	7.413
1.50E−02	13.074	14.200	6.391	7.215	6.514	7.344	6.573	7.398
2.00E−02	12.044	14.282	5.761	7.149	5.861	7.277	5.923	7.333
3.00E−02	9.543	14.056	4.868	6.767	4.917	6.892	4.975	6.955
4.00E−02	7.625	13.226	4.460	6.072	4.478	6.184	4.530	6.251
5.00E−02	6.472	11.845	4.276	5.357	4.278	5.440	4.327	5.506
6.00E−02	5.812	10.237	4.184	4.842	4.178	4.893	4.225	4.954
8.00E−02	5.184	7.604	4.102	4.342	4.089	4.352	4.134	4.404
1.00E−01	4.926	6.167	4.070	4.165	4.053	4.159	4.098	4.207
1.50E−01	4.712	5.002	4.041	4.053	4.022	4.036	4.067	4.082
2.00E−01	4.652	4.744	4.032	4.032	4.013	4.013	4.057	4.058
3.00E−01	4.615	4.628	4.026	4.023	4.006	4.003	4.051	4.047
4.00E−01	4.603	4.602	4.024	4.020	4.003	4.000	4.048	4.044
5.00E−01	4.598	4.593	4.022	4.019	4.002	3.999	4.047	4.043
6.00E−01	4.596	4.589	4.022	4.019	4.002	3.998	4.046	4.043
8.00E−01	4.592	4.585	4.021	4.018	4.001	3.997	4.045	4.042
1.00E+00	4.591	4.582	4.021	4.017	4.001	3.997	4.046	4.041
1.25E+00	4.592	4.581	4.022	4.017	4.002	3.996	4.046	4.041
1.50E+00	4.594	4.581	4.023	4.017	4.002	3.996	4.047	4.041
2.00E+00	4.611	4.594	4.031	4.024	4.012	4.003	4.056	4.048
3.00E+00	4.664	4.652	4.059	4.054	4.041	4.036	4.086	4.080
4.00E+00	4.731	4.730	4.094	4.094	4.078	4.078	4.122	4.122
5.00E+00	4.804	4.816	4.132	4.140	4.118	4.127	4.162	4.171
6.00E+00	4.880	4.904	4.172	4.186	4.160	4.176	4.204	4.220
8.00E+00	5.032	5.076	4.252	4.279	4.246	4.275	4.289	4.319
1.00E+01	5.179	5.232	4.330	4.366	4.329	4.367	4.372	4.409
1.50E+01	5.498	5.550	4.505	4.547	4.515	4.560	4.556	4.601
2.00E+01	5.757	5.783	4.649	4.685	4.668	4.707	4.708	4.746

dominant, and hence, the effective atomic numbers are mainly described by this partial process. In addition, the contribution owing to scattering and pair production processes will be greater in comparison with the photoelectric effect at higher energies. This will influence the effective atomic numbers for both photon energy absorption and photon interaction. Hence, at low energies where the photoelectric effect dominates, the values of $Z_{PEA_{eff}}$ are high; and at higher energies where Compton scattering and pair production processes dominate, the values of $Z_{PEA_{eff}}$ are low. Therefore, the effective atomic numbers vary from a higher value at the region of low energy to a lower value at regions of high energy. The apparent peak in the attenuation properties (μ_{en}/ρ, $Z_{PEA_{eff}}$, and $N_{PEA_{eff}}$) results from the photoelectric effect around the K-absorption edge of Cl. Since none of the biomolecules except for creatinine hydrochloride consist of relatively high-Z constituent elements, the photoelectric effect is not dominant in the attenuation process. Therefore, the effective atomic numbers decrease up to 600 keV without any peaks. The present calculated results resemble the results of Manohara and Hanagodimath [31, 42], who published studies of

Table 3 Effective atomic numbers for photon energy absorption and photon interaction for margaric, tyrosine, inosine, and proline

E (MeV)	Margaric		Tyrosine		Inosine		Proline	
	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$	$Z_{PI_{eff}}$	$Z_{PEA_{eff}}$
1.00E−03	6.378	6.378	7.008	7.008	7.010	7.009	6.912	6.911
1.50E−03	6.399	6.402	7.037	7.038	7.034	7.035	6.940	6.941
2.00E−03	6.410	6.416	7.053	7.056	7.048	7.050	6.955	6.958
3.00E−03	6.414	6.433	7.067	7.078	7.063	7.069	6.968	6.979
4.00E−03	6.399	6.443	7.066	7.091	7.065	7.080	6.966	6.991
5.00E−03	6.363	6.451	7.051	7.099	7.059	7.087	6.950	7.000
6.00E−03	6.306	6.456	7.023	7.106	7.044	7.094	6.920	7.007
8.00E−03	6.120	6.461	6.922	7.115	6.986	7.102	6.815	7.015
1.00E−02	5.844	6.459	6.758	7.119	6.888	7.106	6.644	7.018
1.50E−02	4.956	6.407	6.133	7.098	6.487	7.098	6.004	6.996
2.00E−02	4.190	6.248	5.440	7.016	5.996	7.051	5.310	6.910
3.00E−02	3.412	5.495	4.523	6.559	5.262	6.772	4.416	6.435
4.00E−02	3.133	4.493	4.127	5.770	4.909	6.242	4.038	5.634
5.00E−02	3.020	3.767	3.953	5.011	4.746	5.669	3.873	4.883
6.00E−02	2.965	3.366	3.866	4.493	4.664	5.238	3.791	4.383
8.00E−02	2.917	3.045	3.790	4.012	4.591	4.804	3.719	3.926
1.00E−01	2.898	2.945	3.760	3.847	4.561	4.646	3.691	3.771
1.50E−01	2.881	2.885	3.734	3.744	4.535	4.546	3.665	3.675
2.00E−01	2.875	2.874	3.725	3.725	4.527	4.527	3.657	3.657
3.00E−01	2.871	2.869	3.720	3.717	4.521	4.518	3.652	3.649
4.00E−01	2.870	2.868	3.717	3.714	4.519	4.516	3.650	3.647
5.00E−01	2.869	2.867	3.716	3.713	4.518	4.515	3.649	3.646
6.00E−01	2.869	2.867	3.716	3.713	4.518	4.515	3.649	3.646
8.00E−01	2.868	2.866	3.715	3.712	4.517	4.514	3.648	3.645
1.00E+00	2.868	2.865	3.715	3.711	4.517	4.513	3.648	3.644
1.25E+00	2.869	2.865	3.716	3.711	4.518	4.513	3.649	3.644
1.50E+00	2.870	2.866	3.717	3.711	4.518	4.513	3.649	3.644
2.00E+00	2.876	2.870	3.725	3.717	4.526	4.519	3.657	3.650
3.00E+00	2.896	2.892	3.752	3.746	4.552	4.547	3.683	3.678
4.00E+00	2.921	2.921	3.785	3.785	4.584	4.585	3.715	3.716
5.00E+00	2.949	2.955	3.821	3.829	4.619	4.627	3.751	3.758
6.00E+00	2.979	2.990	3.860	3.874	4.656	4.669	3.788	3.802
8.00E+00	3.040	3.060	3.938	3.965	4.729	4.754	3.864	3.890
1.00E+01	3.100	3.127	4.015	4.049	4.800	4.832	3.939	3.972
1.50E+01	3.241	3.273	4.187	4.228	4.955	4.993	4.107	4.147
2.00E+01	3.362	3.389	4.330	4.366	5.082	5.114	4.247	4.282

$Z_{PEA_{eff}}$ for some amino acids. For creatinine hydrochloride, two different values of $Z_{PEA_{eff}}$ appear at a specific energy owing to the nonuniformity of the mass energy absorption and mass attenuation coefficients. Therefore, two values for each $Z_{PEA_{eff}}$ were obtained at the K-absorption edge of Cl (chloride): one corresponding to the lower side and the other corresponding to the upper side of the same photon energy.

Figure 6 shows the % difference between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ in the energy range of 1–20 MeV for all of the biomolecules studied. It is clear that significant differences exist between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ in the energy region of 10–150 keV for the given biomolecules. Maximum differences up to 45.36% are observed for creatinine hydrochloride at 50 keV. In addition, there is a shift in the corresponding energy positions at which the maximum values of $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ occur for the given biomolecules.

It is worth noting that the considerable discrepancies between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ exist between the transition energies from the photoelectric effect to Compton scattering. The transition energy width between the two extremes is not the same for photon energy absorption and

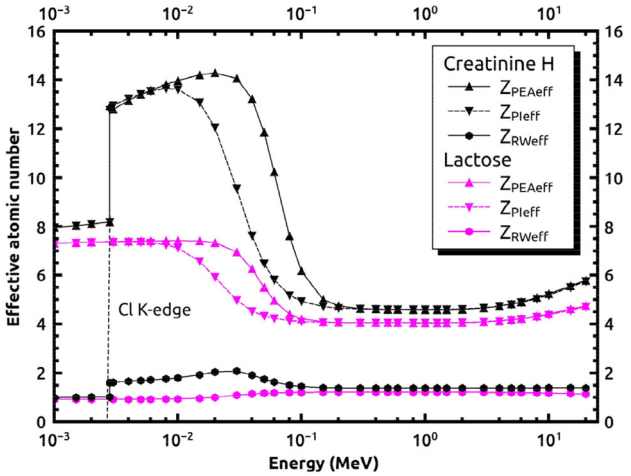

Fig. 2 $Z_{PEA_{eff}}$, $Z_{PI_{eff}}$, and $Z_{RW_{eff}}$ for creatinine hydrochloride and lactose as a function of photon energy

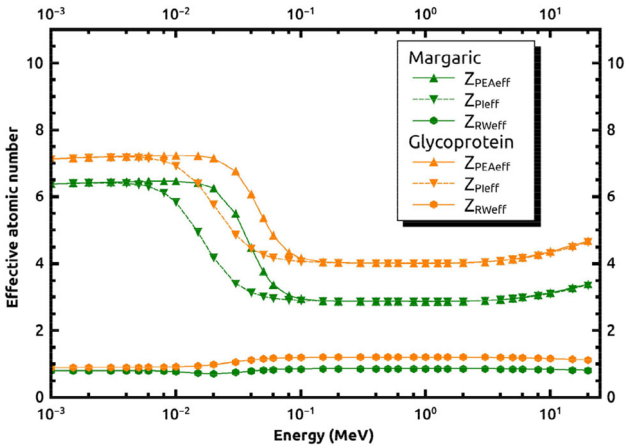

Fig. 3 $Z_{PEA_{eff}}$, $Z_{PI_{eff}}$, and $Z_{RW_{eff}}$ for margaric and glycoprotein as a function of photon energy

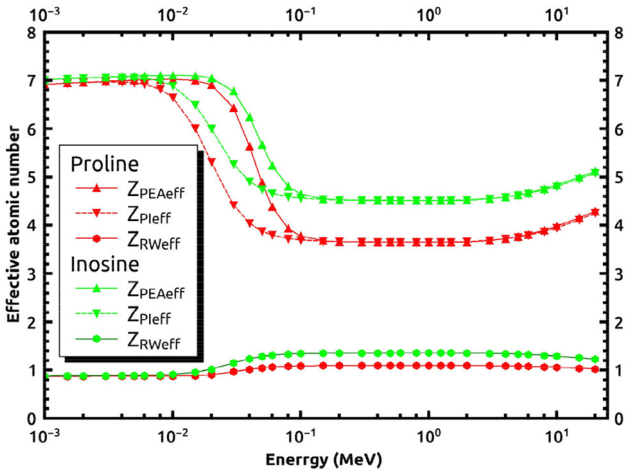

Fig. 4 $Z_{PEA_{eff}}$, $Z_{PI_{eff}}$, and $Z_{RW_{eff}}$ for proline and inosine as a function of photon energy

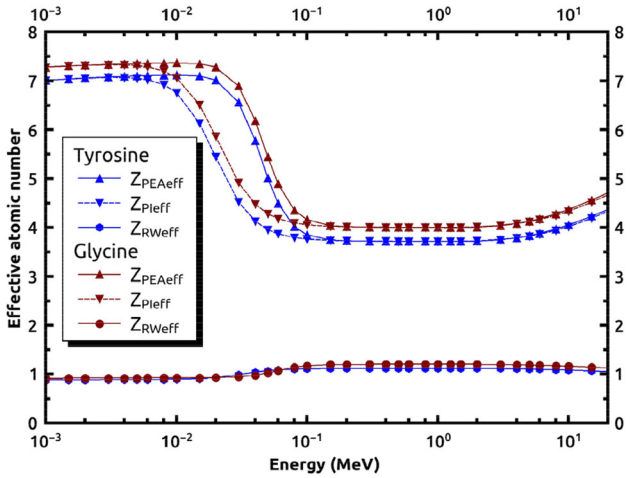

Fig. 5 $Z_{PEA_{eff}}$, $Z_{PI_{eff}}$, and $Z_{RW_{eff}}$ for tyrosine and glycine as a function of photon energy

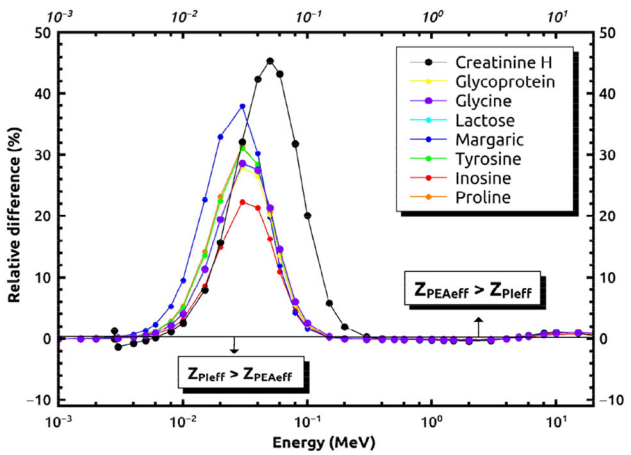

Fig. 6 % difference between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ for biomolecules as a function of photon energy

photon interaction. These ranges of transition energy can be obtained by assuming that the photoelectric effect is dominant at low energies up to where the maximum value of the effective atomic numbers occurs. Compton scattering is dominant at intermediate energies where the value of the effective atomic numbers is almost constant. The energy width that lies between the end of the dominance of the photoelectric effect and the beginning of the dominance of Compton scattering was taken into consideration as a transition energy width between the photoelectric effect and Compton scattering. Therefore, from Fig. 2 in the case of creatinine hydrochloride, it can be seen that the transition energy range for photon energy absorption is from 0.02 to 0.8 MeV, whereas for photon interaction it occurs from 0.008 to 0.8 MeV.

For other biomolecules, the transition energy range between the photoelectric effect and Compton scattering can be discussed in the same manner. Hence, it can be

noted that the transition energy from photoelectric absorption to Compton scattering shifts to higher energies for photon energy absorption (e.g., in the case of creatinine hydrochloride to 20 keV) when compared with photon interaction (e.g., in the case of creatinine hydrochloride to 8 keV). This may occur because (1) the photoelectric effect is dominant for the given biomolecules in the low-energy region, and (2) the photoelectric effect is more important than Compton scattering for photon energy absorption. Given the discrepancies that exist between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$, it could be preferable to use $Z_{PEA_{eff}}$ rather than $Z_{PI_{eff}}$ in medical dosimetry because $Z_{PEA_{eff}}$ represents the absorbed dose [31]. On the other hand, the discrepancies between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ are insignificant ($< 1\%$) below 20 keV and above 200 keV; thus, either $Z_{PEA_{eff}}$ or $Z_{PI_{eff}}$ can be used at these energies.

The relationship between the effective electron density ($N_{PEA_{eff}}$) and $Z_{PEA_{eff}}$ values for the biomolecules is shown in Fig. 7. The variation is smooth and linear because the effective electron densities are directly related to the effective atomic numbers. Likewise, the variation of $Z_{PI_{eff}}$ and $Z_{RW_{eff}}$ as a function of $N_{PI_{eff}}$ and $N_{RW_{eff}}$, respectively, has the same behavior. Thus, the energy dependence of $N_{PEA_{eff}}$, $N_{PI_{eff}}$, and $N_{RW_{eff}}$ is similar to their corresponding effective atomic numbers and can be explained in the same manner. The accuracy of the calculated results of the effective atomic numbers is based on μ_{en}/ρ. The values of μ_{en}/ρ for biomolecule constituent elements were taken from a compilation by Hubbell and Seltzer [9]. Hubbell reported that the envelope of the uncertainty of the mass attenuation coefficient is on the order of 1–2% in the energy range from 5 keV to a few MeV [43]. In the region of energies between 1 and 4 keV, the discrepancies are known to reach a value of 25–50%. In addition, significant discrepancies below 4 keV and new theoretical results of higher accuracy were derived in near-edge soft X-ray regions [44]. In all cases, the calculated results by Eq. 3 are usually considered to be accurate within about 10% of the values that were determined experimentally [45].

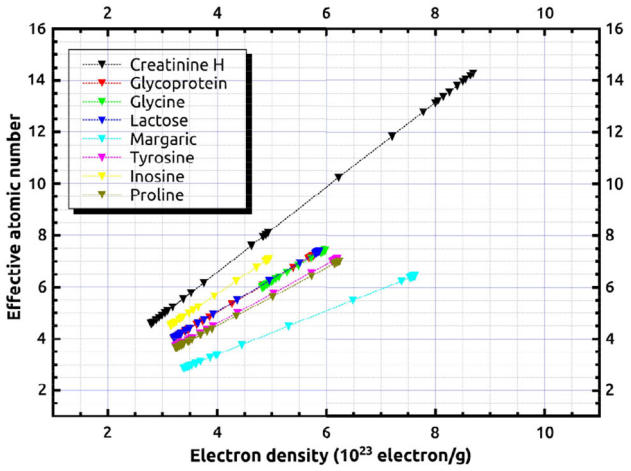

Fig. 7 Effective atomic number ($Z_{PEA_{eff}}$) as a function of effective electron density ($N_{PEA_{eff}}$) for photon energy absorption

4 Conclusion

In this work, photon energy absorption parameters were calculated in the energy region of 1–20 MeV for some biomolecules of dosimetry interest. The variations of the atomic number with the photon energy were attributed to partial photon processes. The existence of relatively high-Z elements in the samples altered the attenuation properties around their own K-absorption edges. Significant differences up to 45.36% were observed between $Z_{PEA_{eff}}$ and $Z_{PI_{eff}}$ in the energy region around 50 keV. Hence, it is recommended to use $Z_{PEA_{eff}}$ rather than $Z_{PI_{eff}}$ for the calculation of absorbed doses in radiation therapy.

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