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RADIATION BEHAVIOR IN BIOLOGICAL COMPOUND: EXPLORING MASS ATTENUATION AND EFFECTIVE ATOMIC NUMBERS FOR GAMMA-RAY INTERACTIONS

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Abstract

This study involved the measurement of mass attenuation coefficients (μ/ρ) for fatty acids across a range of photon energies (from 122 keV to 1330 keV). These measurements were conducted through transmission experiments employing collimated beams generated by 57Co, 133Ba, 22Na 137Cs, 54Mn, and 60Co sources, each producing beams with a diameter of 0.52 cm. The detection of attenuated radiation was achieved using a NaI (Tl) scintillation detector with an energy resolution of 8.2% at 663 keV. The obtained experimental values of (μ/ρ) were subsequently used to calculate the atomic cross-sections (σa), electronic cross-sections (σe), effective atomic numbers (Zeff), and electron densities (Neff). Notably, the study revealed that (μ/ρ), σa, and σe exhibited an initial decrease with increasing photon energy, stabilizing at higher energy levels. In contrast, Zeff and Neff remained relatively constant with changing energy levels. In addition, the research acknowledged that deviations in experimental results for radiological parameters may be influenced by the physical and chemical surroundings of the substances under investigation. Encouragingly, the experimental findings were found to be consistent with values from the WinXCom database, affirming their accuracy and reliability. These outcomes contribute to a deeper understanding of the photon interaction characteristics of these biological substances across diverse energy spectra.

Keywords: *Mass attenuation coefficient, Atomic cross-section, Electronic cross-section, Effective atomic number and, Effective electron density.*

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Introduction

Biological compounds, composed of Carbon, Hydrogen, and Oxygen are complex biomolecules that perform essential physiological functions within living systems. Understanding the interaction of gamma radiations with these compounds is crucial for numerous applications, including medical physics, radiation protection, diagnostics, and radiation therapy. The interaction of γ-rays with matter is influenced by several key parameters, including the mass attenuation coefficients (μ/ρ), effective atomic number (Z_{eff}), and electron density (N_{eff}) [1], [2]. The (μ/ρ) quantifies the likelihood of photon– matter interaction per unit mass of matter per unit area. It provides valuable information about the attenuation characteristics of γ-rays as they pass through different materials. Accurate knowledge of mass attenuation coefficients is crucial for a wide range of scientific and technological applications, including those in biology, agriculture, medicine, and technology [3]. In addition to its significance in radiation-related disciplines, the (μ/ρ) also has implications for understanding the fundamental properties of matter at the atomic and molecular levels. It is used to assess chemical affinity, volatility, and ductility, among other material properties. The determination of accurate photon mass attenuation coefficients, effective atomic number, and electron density is essential for various fields, such as computerized tomography (CT), radiological safety, radiation research, medical diagnosis and treatment, gamma-ray fluorescence investigations, and radiation physics [4], [5].

The Z_{eff} is a parameter that assists in evaluating the suitability of composite materials for specific applications, such as medical radiation dosimetry and radiation exposure [6]. Furthermore, certain elements play crucial roles in biological systems, serving as essential components of metalloenzymes and participating in vital biological functions, such as oxygen transportation, free radical neutralization, and hormone synthesis. The presence of these clinically important elements is necessary for proper physiological functioning. However, variations in the physiological spectrum of individuals can occur due to factors such as dietary deficiencies or excesses, particularly in conditions such as cancer. Obtaining accurate observational data to estimate the mass attenuation coefficients of different materials can be challenging. Experimental studies have been conducted on specific substances, such as fatty acids and mono/disaccharides, using a range of photon energies. These investigations determine effective atomic numbers, mass attenuation coefficients, and electron densities [3], [7]–[9]. For biological samples interacting with photons in the energy range 0.2–1.5 MeV, the mass-energy absorption coefficient of photons has been extensively studied. The WinXCom computer program package, available online, is used for calculations and data analysis.

The present study focuses on determining the Z_{eff}, total atomic cross-section ($б_{Total}$), and N_{eff}. These parameters are primarily derived from the total attenuation factor. Detailed calculations for the mass attenuation coefficients can be found in reference [4], [6], [10]. Specifically, we investigated the properties of psyllid acid at an energy level of 0.0595 MeV. Theoretical values were estimated using the WinXCom program [11], and a comparative analysis was conducted to assess their agreement with the assessed values.

1. Theory

The attenuation of γ-ray pulses as they pass through an absorber is primarily influenced by scattering and absorption phenomena. To accurately estimate the absorption coefficient (μ), the Lamber– Beerr law is commonly employed [12], [13], the law can be expressed as

$$I = I_0 e^{-\mu x} \qquad (1)$$

In Equation (1), I_0 represents the initial strength of the incident γ-ray pulse when no absorber is present in the measurement setup. denotes the attenuated photon intensities of the γ-rays that have penetrated the sample, and its unit is typically given as counts per 50 s. The variable represents the thickness of the sample and is expressed in centimeters. For elements and materials, the experimental attenuation coefficient (μ/ρ) is commonly used to characterize their attenuation properties. (μ/ρ) is represented as [12]

$$\frac{I}{I_0} = e^{-\mu x} \rightarrow \ln\left(\frac{I}{I_0}\right) = -\frac{\mu x \rho}{\rho}$$

$$\therefore \quad \ln\left(\frac{I}{I_0}\right) \times \frac{1}{x\rho} = -\frac{\mu}{\rho} \qquad (2)$$

Where ρ is the sample density($\frac{g}{cm^3}$). $The\ mass\ attenuation\ \frac{\mu}{\rho}$ ($\frac{cm^2}{g}$) (cm^2/g) is specified by Eq. (3) for every chemical mixture:

$$\left(\frac{\mu}{\rho}\right) = \sum_i w_i \left(\frac{\mu}{\rho}\right)_i, \qquad (3)$$

w_i represents the weight percentage of specific component elements within a chemical substance or material. When analyzing the composition of a substance, it is often necessary to identify the relative contributions of its constituent elements. The weight percentage, w_i, provides a quantitative measure of the proportion of the total weight that can be attributed to the ith element. This information is particularly useful in fields such as chemistry, materials science, and industrial processes, where understanding the elemental composition is critical for various applications. The connection between (μ/ρ) and w_i lies in their application in determining the mass attenuation coefficient. The mass attenuation coefficient characterizes how a material attenuates radiation on a per unit mass basis [14]. It considers both the linear attenuation coefficient and the density of the material. By knowing the weight percentage, w_i of each constituent element in a material and the corresponding (μ/ρ) values for those elements, one can calculate the mass attenuation coefficient of the material using appropriate mathematical formulas or tables, so one can say (μ/ρ) represents the normalized linear attenuation coefficient, w_i denotes the weight percentage of a specific element in a substance, and the mass attenuation coefficient is determined by combining these values. This

information is fundamental for understanding the interaction of materials with radiation and has practical implications in fields such as medical imaging, radiation therapy, and material characterization. The fraction by weight w_i of a chemical substance is given by the following formula [15]

$$w_i = \frac{n_i A_i}{\sum_i n_i A_i} \quad (4)$$

XCom, a widely used tool, was employed to determine the mass attenuation coefficients of the investigated materials. The dataset primarily consists of information on the mass attenuation coefficient and the total attenuation cross-section of approximately 100 components. Furthermore, for most datasets, partial cross-section values for incoherent and coherent scattering, photoelectric absorption, and pair output are provided across energies ranging from 1 keV to 100 GeV [18]. To obtain the overall molecular cross-section, σt, an application of a specific relationship is required. This relationship defines the values of the (μ/ρ) and enables the determination of the complete molecular cross-section[16].

$$\sigma_{t,m} = \left(\frac{\mu}{\rho}\right)\frac{M}{N_A} \quad (5)$$

'M' represents the molecular weight, and 'NA' stands for Avogadro's number. When we have the value of the total cross-sectional $б_{Total}$, we can determine it using the following equation [16].

$$\sigma_{t,a} = \frac{1}{N_A}\sum_i f_i A_i \left(\frac{\mu}{\rho}\right)_i = \frac{\sigma_{t,m}}{\sum_i n_i} \quad (6)$$

The formula for calculating the total electronic cross-section $б_{Total}$ for an individual unit involves several variables. The variable fi represents the percentage of element fractional abundance relative to the total number of atoms. The variables n_i and A_i represent the number of formula units and the atomic weight of the component element i, respectively. By applying the following formula, it is possible to determine the $б_{Total}$ for the unit [16].

$$\sigma_{t,\mathrm{el}} = \frac{1}{N_A}\sum_i \frac{f_i A_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i = \frac{\sigma_{t,a}}{Z_{\mathrm{eff}}} \quad (7)$$

The Z_{eff} for each atom in the body is determined by the ratio of the total atomic cross-section ($\sigma_{(t,a)}$) to the total electronic cross-section ($\sigma_{(t,el)}$). This can be expressed as[17]:

$$Z_{\mathrm{eff}} = \frac{\sigma_{t,a}}{\sigma_{t,\mathrm{el}}} \quad (8)$$

The effective atomic number represents the average atomic number experienced by the incident radiation as it interacts with the atoms in the body. It takes into account both the atomic cross-section, which describes the probability of interaction with the nucleus, and the electronic cross-section, which describes the probability of interaction with the electrons

surrounding the nucleus. The larger the value of Z_{eff}, the greater the overall interaction of the incident radiation with the atoms in the body. The following equation provides the expression for the effective density of electrons or N_{eff} in units of electrons per gram (electron/g). It is calculated using the following formula:

$$N_e = \frac{(\mu/\rho)}{\sigma_{t,\mathrm{el}}} = \frac{N_A}{M} Z_{\mathrm{eff}} \sum_i n_i = \frac{N_A Z_{\mathrm{eff}}}{\langle A \rangle} \qquad (10)$$

In this equation, μ represents the linear attenuation coefficient, ρ represents the density of the material, N_A is Avogadro's number, M is the molar mass, Z_{eff} is the effective atomic number, and $\sum_i n_i$ represents the sum of the number of formula units for each component element. To identify compound A, one can calculate the percentage of its molecular weight (M) divided by the total number of atoms of all forms present in the sample[18]. This percentage is given by:

$$\langle A \rangle = \frac{\mathrm{M}}{\sum_i n_i} \qquad (11)$$

the value ⟨A⟩ represents the average molecular weight per atom, which can be used to determine the composition of compound A.

2. Experimental and measurements

In the experimental setup described, psyllid acid was used as the fatty acid sample for the transmission experiment. The sample was weighed using a digital electric balance, and the weighing process was repeated four times to ensure consistency in the mass measurement. The energy range up to 1500 keV was chosen for the experiment because it is commonly used in various fields such as radiation biology, industry, and dosimetry [19][20]. Photons in the keV range are particularly relevant to medical diagnostics and therapeutic applications. Radiation sources including ^{57}Co (122 keV), ^{133}Ba (356 keV), ^{137}Cs (662 keV), ^{60}Co (1170 and 1330 keV), ^{22}Na (511 and 1275 keV), and ^{54}Mn (840 keV) were used to irradiate the organic compounds. A NaI (Tl) scintillation detector with an energy resolution of 8.2% at 663 keV was used to measure photon intensities in a narrow beam setup with good geometry. The experimental arrangement and geometry details are shown in Figure1.

To minimize background counts, a background spectrum was collected for a duration of 3 h, and the counts were found to be relatively constant (30745±133). An extrapolation technique was employed to determine the background counts by selecting two channels on each side of the photo peak and summing their counts. In addition, a 5-cm- thick lead shield was used to cover the detector and the surroundings of the experimental setup, reducing the detection of scatter or background radiation from other sources and the environment.

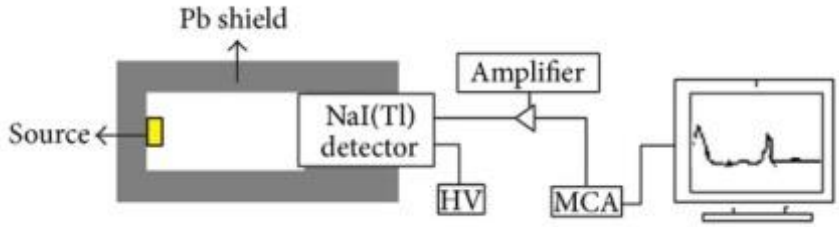

Figure 1. Low level background gamma-ray-spectrometer diagram [21]

A distance between 30 and 50 cm was maintained between the source and detector to ensure that the maximum scattering angle remained below 30 min. The thickness of the compounds was measured using a traveling microscope, and the uncertainty in the thickness measurement was within 0.3%. The compound's mass thickness ranged from 0.200 g.cm^{-2} to 0.450 g. cm^{-2}, selected to satisfy the ideal condition of $2 \leq ln(I_0/I) \leq 4$ as much as possible. The uncertainty in the mass per unit area measurement was within 0.5%. To minimize statistical uncertainty in the measured counts, an optimum count rate (10^4-10^5) and a counting time of 900 s were chosen. This helped mitigate the pulse pile-up and multiple scattering effects. The non-uniformity of the compounds was checked by exposing them to the incident beam, and the error due to non-uniformity for all energies was found to be less than 0.05%.

The buildup of the photon dose is influenced by energy, target thickness, and atomic number. In this experiment, a detector with good energy resolution, a narrow beam geometry setup, and an appropriate thickness range were selected to minimize the dose buildup, considering it to be negligible. The experimental uncertainty in the measured mass attenuation coefficient depends on the uncertainties in the thickness and mass measurements of the compounds. The uncertainties in both I (attenuated intensity) and I_0 (unattenuated intensity) can also affect the results [22]; however, they were measured with good statistics (< 1%). The main sources of error in the measurement of mass attenuation coefficients in this work are counting statistics (<5%), non-uniformity (<0.05%), and mass per unit area (<0.5%) of the compounds. These errors arise from deviations in the measurement of the attenuated and unattenuated intensities and the thickness and mass measurements of the compounds.

3. The Results and Discussion

Table 1 enumerates the atomic number and chemical formula pertaining to the specimen under investigation. Table 2 presents the experimental and predicted value of (μ/ρ) for psyllid acid. The graphical representation in figure 2 illustrates the energy-dependent behavior of these values. It is evident from the figure that (μ/ρ) is influenced by both photon energy and chemical composition. Specifically, the (μ/ρ) values of organic compounds exhibit a decreasing trend up to 1170 keV, after which they tend to stabilize at higher energies.

Notably, the experimental values, as depicted in table 2 and figure 2, exhibit consistency with the predicted values derived from the WinXCOM database, considering the experimental uncertainties. These uncertainties may arise due to the effects of chemical, molecular, and thermal environments on (μ/ρ) [23]. Figure 3 which present typical plots of σ_{Total} (absorption cross section and elastic scattering cross section), it becomes evident that decrease as the energy increases. This behavior is similar to that observed for (μ/ρ). By employing the experimental and predicted values of (μ/ρ), Z_{eff} was determined using Equation (8) and is listed in table 4 and illustrated in figure 4 for both experimental and predicted values. The trend of Z_{eff} as a function of energy indicates a nearly constant behavior, primarily attributed to the linear Z-dependence of incoherent (Compton) scattering, which is the dominant process at present energies. Furthermore, the values of Z_{eff} are found to be approximately equal to the mean atomic number. Table 5 and figure 5 provides the results of N_{eff} along with their corresponding experimental uncertainties, demonstrating the nearly energy-independent nature of N_{eff} . In the transmission experiment, meticulous measures were undertaken to minimize uncertainty. A parallel narrow beam of photons was directed onto the compounds, and the uncertainties in photon intensity measurements (I and I_O) were estimated to be less than or equal to 1%. Moreover, the ratio of experimental to predicted values was observed to be less than or equal to 5%.

Table 1: show the sample formula

sample	Chemical formula	atomic weight number	Effective atomic weight number
Psyllic acid	$C_{33}H_{66}O_2$	494.889	4.900

Table 2: show a comparison of calculated and theoretical values of (μ/ρ). Deviation= [(theory - experiment)/theory] *100% [24][25]

source	Energy keV	(μ/ρ)		deviation
		Theo.	Exp.	
^{57}Co	122	0.1617	0.1585	2%
^{133}Ba	356	0.1131	0.1074	5%
^{22}Na	511	0.0978	0.0939	4%
^{137}Cs	662	0.0874	0.0830	5%
^{54}Mn	840	0.0783	0.0767	2%
^{60}Co	1170	0.0667	0.0633	5%
^{22}Na	1275	0.0638	0.0612	4%
^{60}Co	1330	0.0624	0.0605	3%

Table 3. Displays the experimental and theoretical total cross-sections, measured in barns per atom.

source	**Energy (keV)**	**б Total**		**deviation**
		Theo.	Exp.	
^{57}Co	122	132.882	130.225	2%
^{133}Ba	356	92.9436	88.2964	5%
^{22}Na	511	80.3539	77.1397	4%
^{137}Cs	662	71.7991	68.2092	5%
^{54}Mn	840	64.3538	63.0667	2%
^{60}Co	1170	54.7800	52.0410	5%
^{22}Na	1275	52.4133	50.3168	4%
^{60}Co	1330	51.2875	49.7488	3%

Table 4. Provides the values of the effective atomic number.

source	Energy (keV)	Z_{Effect}
^{57}Co	122	2.2323
^{133}Ba	356	2.2737
^{22}Na	511	2.2878
^{137}Cs	662	2.2980
^{54}Mn	840	2.3074
^{60}Co	1170	2.3205
^{22}Na	1275	2.3239
^{60}Co	1330	2.3256

Table 5. Provides electron densities in electrons per gram (electrons/g) for the sample.

source	Energy (keV)	Ne 10^{24} electrons/g
^{57}Co	122	0.2744
^{133}Ba	356	0.2794
^{22}Na	511	0.2812
^{137}Cs	662	0.2824
^{54}Mn	840	0.2836
^{60}Co	1170	0.2852
^{22}Na	1275	0.2856
^{60}Co	1330	0.2858

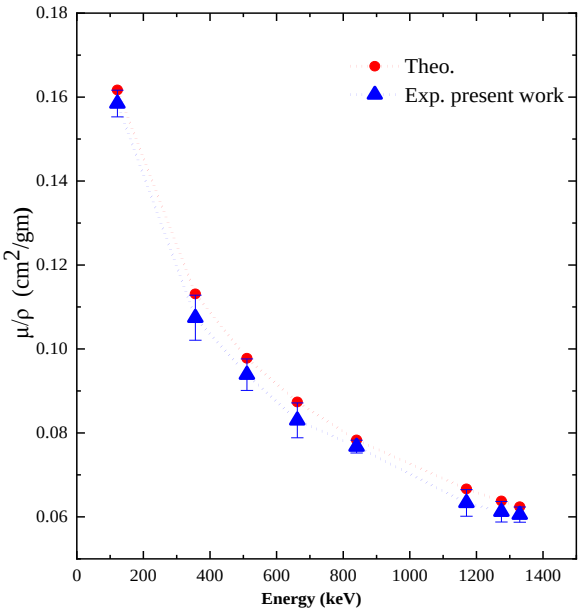

Figure 2 depicts the relationship between μ/ρ and energy in keV.

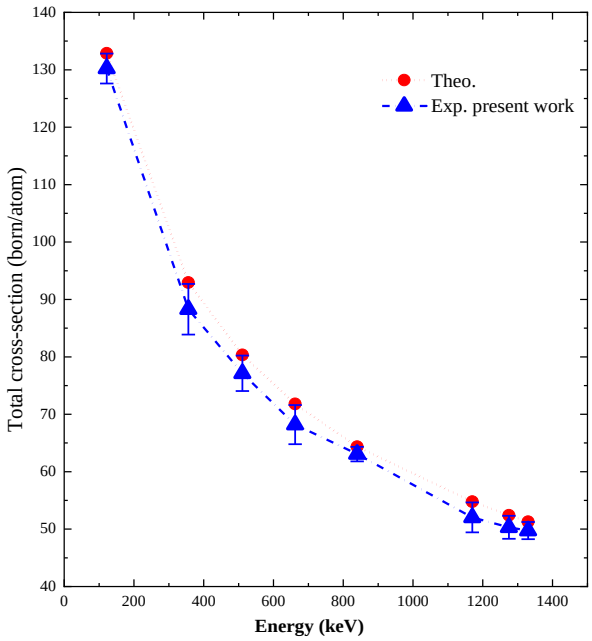

Figure3. Illustration to compare the theoretical and practical σ_{Total} values calculated for the current work & Energy from 0.122 to 1.33 MeV.

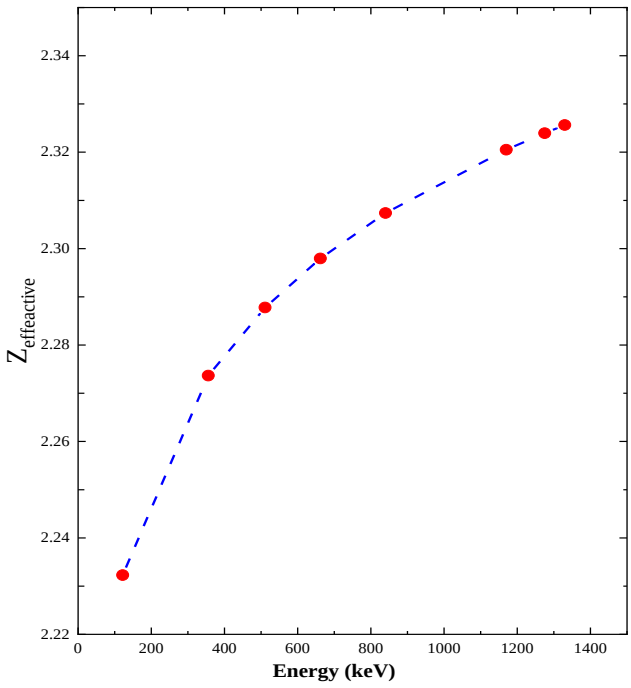

Figure4. Plot of Z_{effe} atomic number &Energy from 0.122 to 1.33 MeV

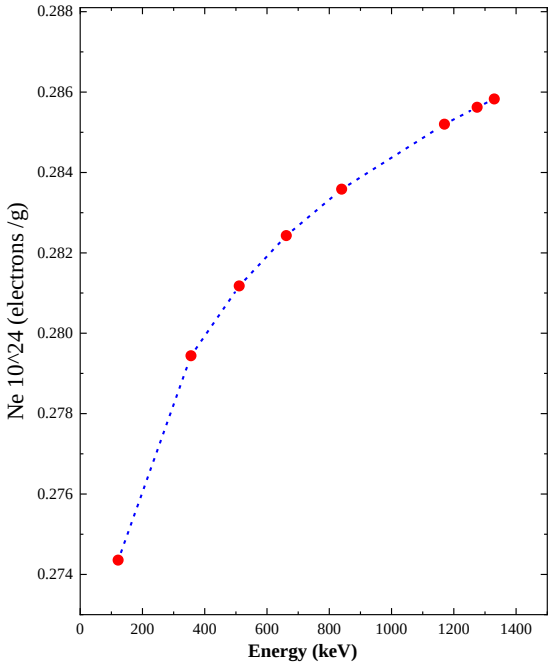

Figure5. Plot of ($N_{effective}10^{24}$) Effective Electron densities (electron/g) & Energy from 0.122 to 1.33 MeV

4. Conclusion

The experimental investigation of the psyllic acid sample has provided valuable insights into the determination of Z_{eff}, $б_{Total}$, and N_{eff} parameters through their dependence on (μ/ρ). Particularly for biological compounds composed of Hydrogen (H), Carbon (C), and Oxygen (O), the physical quantity (μ/ρ) has proven to be a sensitive and informative measure for assessing the Z_{eff}, $б_{Tota}$, and N_{eff} parameters characteristics of such compounds. Notably, the (μ/ρ) values exhibit a dependence on the physical and chemical environments surrounding the samples, highlighting the influence of these factors on photon-matter interactions. An important observation is that the values of (μ/ρ) decrease as the energy of incident photons increases, a trend that is mirrored by the variations in $б_{Total}$. Furthermore, the N_{eff} parameter is closely linked to Z_{eff}, displaying a similar energy dependency. These findings significantly contribute to our understanding of how (μ/ρ) values evolve when Z_{eff} and N_{eff} values undergo changes, specifically in the context of biological molecules like fatty acids that predominantly consist of H, C, and O. Another noteworthy aspect of the study is the correlation between the Z effective values of the sample and their effective atomic weights within the relevant energy range. Additionally, the consistency of electron densities across all energies implies a stable number of electrons per gram of sample engaged in photon interaction. This observation suggests that incoherent scattering largely accounts for the total attenuation cross-sections within this energy range.

In summary, the experimental investigation of the psyllic acid sample has shed light on the interplay between (μ/ρ) values, Z_{eff}, $б_{Total}$, and N_{eff} parameters. The results highlight the significance of physical and chemical environments in determining the (μ/ρ) values, and their impact on photon-matter interactions in biological compounds. The study's findings contribute to the broader knowledge of these compounds and provide valuable insights for future research and applications in related fields.

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