Calculate Effective Atomic Number, Mass and Cross-Section Attenuation Coefficients for Nonanoic Acid by Using Gamma-Ray Sources

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Abstract

The effective atomic number ($Z_{effective}$), total atomic cross-section ($б_{Total}$) electron density ($N_{effective}$) have been Measured depending on the mass attenuation coefficient (μ/ρ). By using Gamma-ray radiation (γ), emitted from sources ($57Co, 133Ba, 22Na, 137Cs, 54Mn, and\ 60Co$) with energies from ($0.122, 0.356, 0.511, 0.662, 0.84, 1.17, 1.275\ and\ 1.33MeV$) respectively. using the Sodium Iodide Scintillation Detectors NaI (Tl) at 662 keV and resolution about 8.2% have been measured the mass attenuation coefficients for the sample "Nonanoic acid its common name Pelargonic acid" it's chemical formula $C_9H_{18}O_2$. The data from the mass attenuation coefficient were then employed to study $Z_{effective}$, $N_{effective}$, and $б_{total}$ of the sample. In the presence of gamma-ray energy, it was discovered that the effective atomic number and effective electron densities first drop and they tend to remain nearly constant. The experimental values obtained by $Z_{effective}$ and $N_{effective}$ were in excellent agreement with the theoretical values. The theoretical data that is accessible is obtained from XCom, which is available online. The study's findings aid in understanding how (μ/ρ) values change when Z_{eff} and N_{eff} values vary in the case of H, C, and O based biological molecules such as fatty acids.

Key Words: Sodium Iodide Scintillation Detectors, Effective Atomic Number, Total Atomic Cross Section, Effective Electron Density.

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Introduction

The penetration of γ-rays in matter relies on the mass attenuation coefficient (μ/ρ), effective atomic number ($Z_{effective}$), and electron density ($N_{effective}$). The (μ/ρ) reflects the likelihood of photon-matter interaction for a region with a unit mass of matter per unit area. Although the awareness of the mass attenuation coefficients of γ-ray in biological and other relevant materials is essential for technological, biological, agricultural, and medical purposes (Kucuk et al., 2012), Assignments for biological, agricultural, and medical objectives are also quite important in this regard. Can be used to find other matter properties at the molecular and atomic levels (Talib et al., 2020) (Hussein Faraj et al., 2019). In addition to communicating around fundamental matter properties at the scale of atomic, this coefficient (μ/ρ) is also used to determine chemical affinity, volatility, and ductility in addition to its other applications.

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Obtaining accurate photon mass attenuation coefficients, effective atomic number, and electron density is essential for many applications including computerized tomography (CT), radiological safety, in research, diagnosis, and treatment by radiation, gamma-ray fluorescence investigations, and radiation physics, among other areas of study (Jawad Al-Hamzawi et al., 2020)(Alabood et al., 2019). And in this study article, we will mostly depend on it to compute the coefficients ($Z_{effective}$, $N_{effective}$, $б_{Total}$) which will be discussed later in section 4.

The effective atomic number is helpful in evaluating whether a composite material that has appropriate properties For dosimeter of medical radiation, the dose unit should be used in lieu of a particular quantity of energy., as well as in dosimeter for measuring the quantity of radiation exposure (Manjunathaguru & Umesh, 2006).

For the organism to function correctly, a great percentage of clinically critical elements are also required. These components make up the majority of metalloenzymes and are essential to important biological functions, such as transporting oxygen, neutralising free radicals, and inducing hormone production. The physiological spectrum of some patients to certain conditions, such as cancer, falls short or exceeds the physiological spectrum of humans in terms of bio-medical aspects (such as dietary deficits or excesses (Tonguc et al., 2018).

It is hard to identify several observational data linked to estimating mass attenuation coefficients of multiple samples that could be found in the literature. Experiments have been performed on certain fatty acids with an energy spectrum of 0.122-1.330 MeV to get effective atomic numbers, mass attenuation coefficients, and electron densities (Hadi et al., 2021) (Yahya Hadi et al., 2021). Measurement of the mass attenuation coefficients for mono and disaccharides has been completed at photon energies of 0.008136, 0.013596, 0.017781, 0.22581, and 0.32890 MeV (Han & Demir, 2010) (Kore & Pawar, 2014). For biological samples that consume photons in the energy spectrum of 0.2–1.5 MeV, The mass energy absorption coefficient of photons has been determined. personal computer program package WinXCom al so available online is used to run calculations and to associate measurements with each other (Berger et al., 1987). The present research determined the effectual atomic number $Z_{effective}$, as well as the total atomic cross-section $б_{Total}$, and effectual electron density $N_{effective}$, relying primarily on the total attenuation factor (one can see the reference (Yahya Hadi et al., 2021) for the details of calculating the mass attenuation coefficient in detail, but it will be clarified remain parameters in this research). We used these findings for Nonanoic acid, which has energy of 0.0595 MeV, in our work. We estimated theoretical values using WinXCom and have contrasted those assessed values to see how they matched.

Theory

An absorber reduces the strength of a γ-ray pulse as it passes thru it. Attenuation degree is highly influenced by scattering and absorption, to varying degrees to estimate the absorption coefficient μ, Lambert-Beer law must be added (Akça & Erzeneoɨlu, 2014; Jawad Al-Hamzawi et al., 2020).

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

Where, (I_0) has the strength of the γ-ray incident when the amount is not used in the measurement, (I) is attenuated photon intensities of rays penetrating the sample the unit used for this quantity is (count/50 second), and (x)in unit of centimetre refer to sample thickness. For elements, the experimental attenuation coefficient (μ/ρ) is represented as (Gagandeep et al., 2000)(Apaydin et al., 2009).

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

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

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:

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

In this case, $\frac{\mu}{\rho}$ is defined before, and w_i is defined as the percentage of the ith component element's weight in the total. Because $\frac{\mu}{\rho}$ does not depend on the process of the material, it is helpful for determining the mass attenuation coefficient. The fraction by weight w_i of a chemical substance is given by the formula (Gowda et al., 2005) (Al-Sharifi et al., 2018).

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

XCom was used to determine the mass attenuation coefficients of the materials involved. The bulk of data sets contain information on the mass attenuation coefficient and the overall attenuation cross-section of about 100 components. Additionally, for the bulk of data sets, partial cross sections for incoherent and coherent scattering, photoelectric absorption, and pair output are provided at energies ranging from 1 keV to 100 GeV (Demir et al., 2012). σ_t is to apply the relationship which specifies the values of the mass attenuation coefficients in order to find the whole molecular cross-section:

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

In where M is the weight of a molecule and N_A denotes the number of Avogadro calculations. When the total cross-sectional б $_{Total}$ is known, it may be computed using the following equation: (Sandhu et al., 2002)

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

Where f_i corresponds to percentage of the element i's fractional abundance in relation to the total number of atoms, The variables n_i and A_i relate to the number of formula units and the atomic weight of the component element i respectively, in the formula. It is possible to calculate the total electronic cross-section б $_{Total}$ for an individual unit by using the following formula (Sandhu et al., 2002):

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

For each atom in the body, there is both an atomic and electronic cross-section. The cross-section is proportional to the (Z $_{effective}$) atomic number as shown:

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

Or

The value of Z effect, it is find from equation (Manjunathaguru & Umesh, 2006):

$$Z_{effect} = (0.28) \times (E)^{\mathbf{0.092}} \times \left(A_{effect}\right)^{(\mathbf{1.329 - 0.0471 \times ln(E)})} \quad (9)$$

Where; E the energy of source effect upon sample in MeV and (A $_{effect}$) is calculate as: A_{effect} = A divided by total number of molecule, A is atomic weight of component.

Eq. (10) yields the efficient density of electron or efficient number of electron $N_{e,}$ which denoted to electrons number in unit (electron/g) (Tonguc et al., 2018) (Kore & Pawar, 2014):

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

Compound A may be identified by the proportion of its molecular weight that is divided by the total number of atoms of all forms that are present in the sample. This percentage can be calculated:

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

Operation of Experimental and Measurements

In the current inquiry, it used $57Co, 133Ba, 22Na, 137Cs, 54Mn, and\ 60Co$. The radioactive sources supplied radiation with energies of "0.122, 0.360, 0.511, 0.662, 1.170, 1.275, and 1.330 MeV, which were oriented and identified using a NaI (Tl) detector. A Geiger counter detected the sensor's radiation, which was then intensified and analyzed using an 8K multichannel analyzer. Pelleted (uniform thicknesses about 0.17 g/cm^2) the sample granules were placed inside a plastic container in a coordinated and tight shape, the sample for which was taken and subjected to an inspection on the Nonanoic acid under investigation. The observed negligible photons attenuation in the blank container indicates it is a distance to the middle of the containers, as is suspected. Before each sample was placed in the device, it was accurately weighed using a digital balance with an accuracy of close to 0.001 mg. when a mass was measured; it was performed a variety of times to achieve a reliable value. The weight of the sample was determined by taking the mean of this series of values. We were able to calculate the diameter of the pellet by determining the mass per unit area, and we were able to calculate the overall mass by measuring the mean value of the particle's mass.

In order to compute the photon energy that were incident and transmitted, a camera with monochromatic white light filters is needed. A narrow beam setup was introduced. One can show in (Fig: 1) the graphical representation of the experimental set's structure. The coefficients (μ/ρ) for "Behenic" fatty acid sample were determined experimentally as indicated in the figures in the results section and theoretically using Equation 3. Using xcom, values of coefficients (μ/ρ) for all currently used photon energies were also

calculated. Other reasons that could cause errors due to the participation of small-angle scattering were taken into account, such as different types of background scattering, sample impurities, sample irregularity, image construction results, and dead time of the counting instrument. And by adopting the calculated values of attenuation coefficients the rest of the parameters were found and studied.

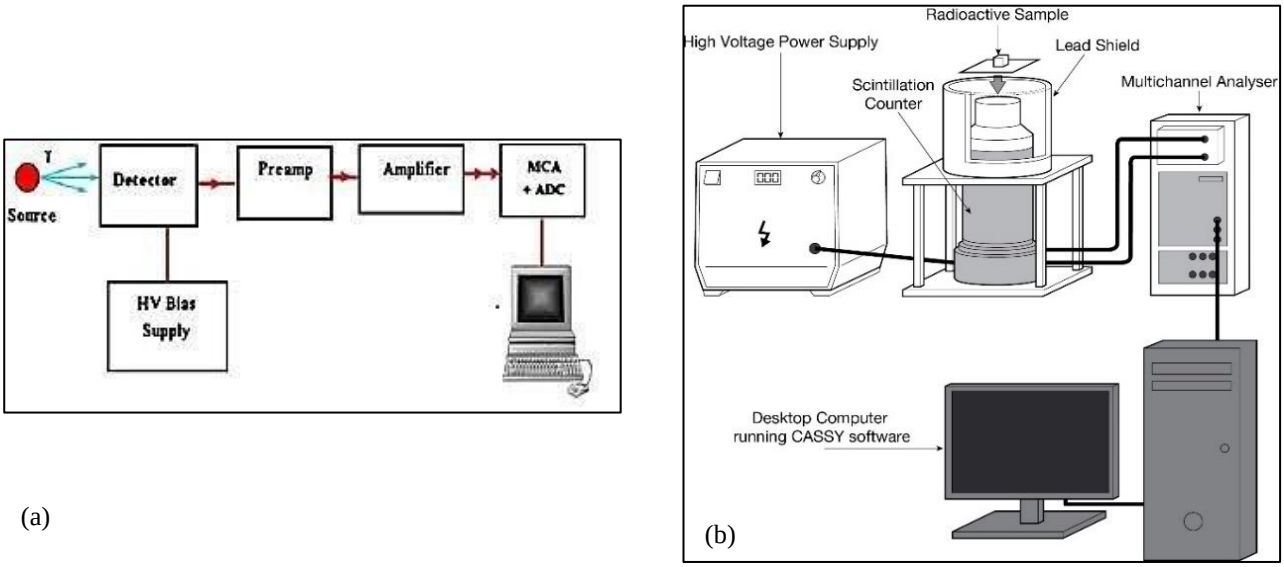

Figure 1. (a) low level background gamma-ray-spectrometer diagram (b) Scintillation counter as a spectrometer (Hadi et al., 2021).

The Findings and Discussion

The atomic number and chemical formula of the sample under study are listed in Table 1, whereas Table 2 It includes comparing the results of the experiment with the theoretically calculated values obtained through the Xcom database "mentioned previously" about the mass attenuation coefficients. The coefficient (μ/ρ) is obviously dependent on energy of incident photon and chemical composition, with photon energy and chemical composition having a direct effect on the values of (μ/ρ) of Nonanoic acid see Fig.2a. Tables 3, 4 provide an expanded list of the Nonanoic's ($б_{Total}$), ($N_{effective}$), and ($Z_{effective}$). According to the results in Fig. 2b, as photon energy rises, the cross-sections decrease. This finding indicates that the sample has a broad range of elements with atomic numbers ranging from H (30.82 eV) to O (1,408.01 keV), and therefore the total of electrons per atom during photon interaction with the sample is rather constant. This serves as a reminder that molecules combining hydrogen, carbon, and oxygen may act as incoherent scatters. When photons and a certain chemical substance are present, the quantity of Nel is very dependent on the total of photons and the chemical concentration, can see the effect of gamma-rays on Z $_{effective}$), and ($N_{effective}$) of the sample in Fig.2c, 2d.
Both the background removal and peak fitting techniques exhibit faults, resulting in inaccurate estimates. To carry out the calculation of cross-sections of photon–atom interactions are taken into consideration in these computations. For this reason (Tables 2,3), the experimental values found in this work are quite close to those predicted by theory.

Table 1. Show the sample formula

sample	Chemical formula	atomic weight number	Effective atomic weight number
Nonanoic acid	$C_9H_{18}O_2$	158.241	5.457

Table 2. Comparison of calculated and theoretical mass attenuation coefficients for the sample, Deviation= [(theory - experiment)/theory] *100%

source	Energy MeV	(μ/ρ)		deviation
		Theo.	Exp.	
$57Co$	0.122	0.159	0.153	4%
$133Ba$	0.356	0.111	0.116	-4%
$22Na$	0.511	0.096	0.101	-5%
$137Cs$	0.662	0.086	0.082	5%
$54Mn$	0.84	0.077	0.074	4%
$60Co$	1.17	0.066	0.062	5%
$22Na$	1.275	0.063	0.060	5%
$60Co$	1.33	0.061	0.058	6%

Table 3. The experimental & theoretical total cross-sections barn/atom of sample

source	Energy MeV	6 Total		deviation
		Theo.	Exp.	
57*Co*	0.122	41.859	40.184	4%
133*Ba*	0.356	29.220	30.388	-4%
22*Na*	0.511	25.257	26.520	-5%
137*Cs*	0.662	22.569	21.440	5%
54*Mn*	0.84	20.228	19.419	4%
60*Co*	1.17	17.216	16.356	5%
22*Na*	1.275	16.475	15.652	5%
60*Co*	1.33	16.121	15.153	6%

Table 4. Values of Effective atomic number, and Electron densities in (electrons/g) of the sample

source	Energy MeV	Z Effect.	Ne 10^24 electrons /g
57Co	0.122	2.6031	0.2873
133Ba	0.356	2.6370	0.2910
22Na	0.511	2.6485	0.2923
137Cs	0.662	2.6568	0.2932
54Mn	0.84	2.6645	0.2941
60Co	1.17	2.6752	0.2952
22Na	1.275	2.6779	0.2955
60Co	1.33	2.6793	0.2957

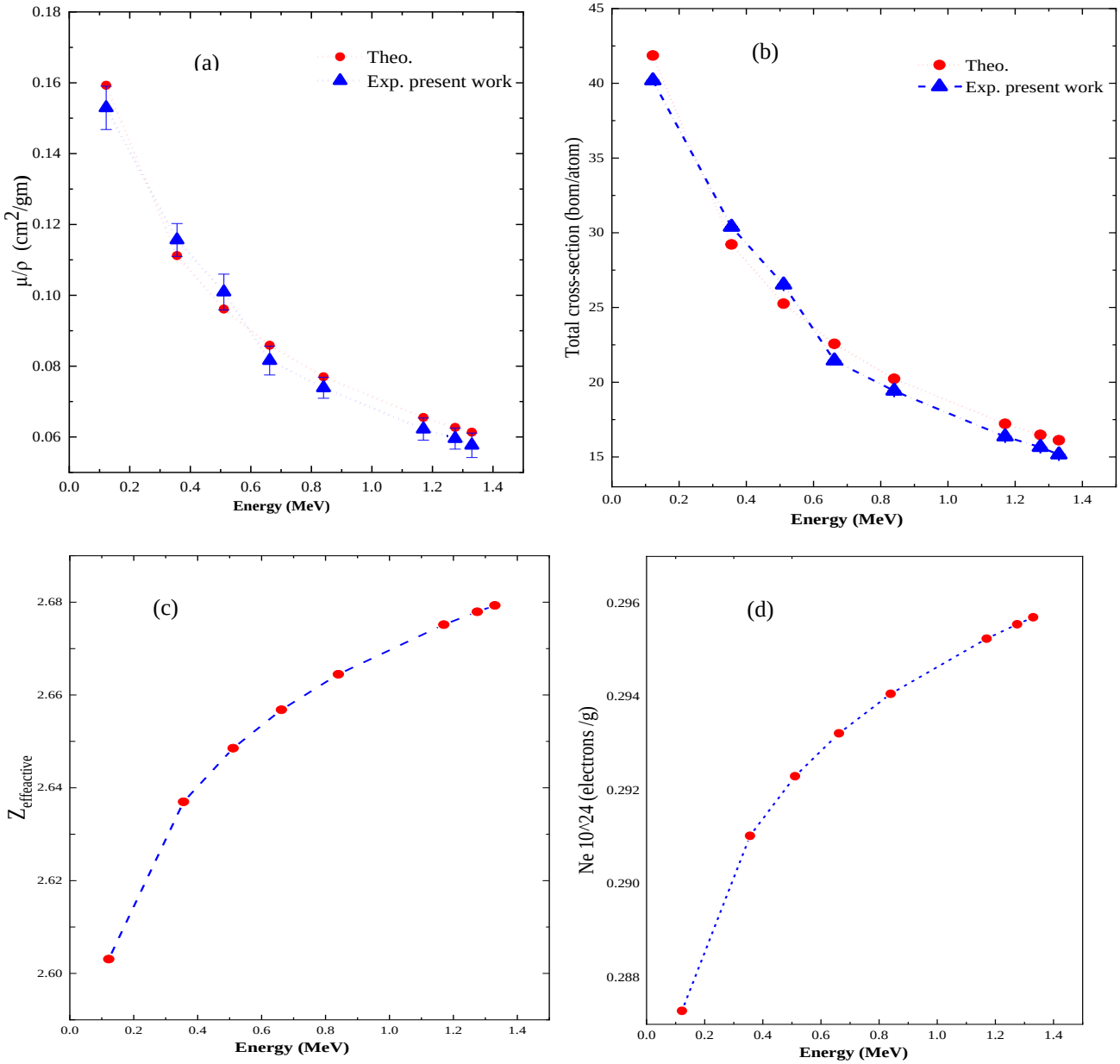

Figure 2. Plot Illustration for (a) Compare the theoretical and practical (μ/ρ) values calculated for the current work & energies from 0.122 to 1.33 MeV. (b) Compare the theoretical and practical (6 Total) values calculated for the current work & Energy from 0.122 to 1.33 MeV. (c) The behavior of Z effective values at energies from 0.122 to 1.33 MeV. (d) Illustration electron densities (electron/g) at energies from 0.122 to 1.33 MeV

Conclusion

The Nonanoic acid sample was subjected to experimental research to determine parameters $Z_{effective}$, $б_{Total,}$ and $N_{effective}$ by depended on (μ/ρ). For H, C, and O based biological compounds, it has been noticed that the (μ/ρ) physical quantity is a helpful and sensitive physical quantity for determining the $Z_{effective}$, $б_{Total,}$ and $N_{effective}$ of the compounds. The values of (μ/ρ) during the photon interaction with matter are dependent on the physical and chemical environments in which the samples are situated. The (μ/ρ) values were found to decrease as the photon energy rose. $б_{Total}$ has the same variance as (μ/ρ) values. $N_{effective}$ is intimately linked to $Z_{effective}$, and their energy dependency is identical. The study's findings aid in understanding how (μ/ρ) values change when $Z_{effective}$ and $N_{effective}$ values vary in the case of (H, C, and O) based biological molecules such as fatty acids. The fact that the $Z_{effective}$ values of the sample utilized in this study are linked to their effective atomic weights in the energy region of interest is also worth mentioning in this context. It is implied from the consistency of electron densities for the sample at all energies that the number of electrons per gram of sample engaging in photon interaction with the sample is stable, This implies that incoherent scattering accounts for almost all of the total attenuation cross-sections in this energy range. At the energies of interest, the $Z_{effective}$, $б_{Total}$, and $N_{effective}$ values are consistent with the other data that is currently available.

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