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Measurement of attenuation cross-sections of some fatty acids in the energy range 122–1330 keV

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Abstract. The mass attenuation coefficients (μ_m) have been measured for undecylic acid ($C_{11}H_{22}O_2$), lauric acid ($C_{12}H_{24}O_2$), tridecylic acid ($C_{13}H_{26}O_2$), myristic acid ($C_{14}H_{28}O_2$), pentadecylic acid ($C_{15}H_{30}O_2$) and palmitic acid ($C_{16}H_{32}O_2$) using ^{57}Co, ^{133}Ba, ^{137}Cs, ^{60}Co and ^{22}Na emitted γ radiation with energies 122, 356, 511, 662, 1170, 1275 and 1330 keV, respectively. The accurate values of the effective atomic number (Z_{eff}), atomic cross-section ($\sigma_{t,}$), electronic cross-section (σ_e) and the effective electron density (N_{eff}) have great significance in radiation protection and dosimetry. These quantities were obtained by utilizing experimentally measured values of mass attenuation coefficients (μ_m). A NaI(Tl) scintillation detector with 8.2% (at 662 keV) resolution was used for detecting of attenuated γ-photons. The variation in Z_{eff} and N_{eff} of fatty acids with energy is discussed. The experimental and theoretical results are in good agreement within 2% deviation.

Keywords. Fatty acids; NaI(Tl) scintillation detector; Z_{eff} and N_{eff}.

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1. Introduction

Radioactive isotopes are widely used in different fields such as radiation protection, radiation therapy, agriculture, medicine, industry and research. Data on the absorption and scattering of X-rays and γ-photons in the biological system have been used in medical physics and radiation biology [1]. Biologically important systems such as carbohydrates, amino acids, fatty acids and proteins are the building blocks of human body and other living systems. These complex biomolecules are necessary for the body to function and are responsible for various physiological functions inside the living system. Hubbell [2] has carried out comprehensive theoretical studies on the interaction of γ-rays, and has reported that the energy range 5–1500 keV has tremendous application in diagnostic radiology.

The mass attenuation coefficient (μ_m) is the basic parameter for understanding the absorption and scattering of X-ray and γ-ray photons in matter, and can be defined as a measure of the probability of interaction between incident photons and sample of mass per unit area. Similarly, the mass energy absorption coefficient (μ_{en}) is a measure of imparted interacting photon energy to kinetic energy of charge particles, and can be calculated directly by employing sphere transmission method [3]. The mass energy absorption coefficient can be utilized for calculating the absorbed dose, which is useful in radiotherapy [4]. Hubbell and Seltzer [5] have given tables of μ_m and μ_{en} for some elements and materials of dosimetric interest as these are the basic parameters for calculating the penetration of γ-ray photons in an absorber. The values of mass attenuation coefficient (μ_m) derived from X-rays and γ-photons are valuable in radiation biology, dosimetry, etc. [2]. Similarly, scattering cross-section data for various interaction processes have potential applications, including the area of radiation shielding, industrial irradiation and monitoring, crystallography and X-ray spectroscopy, besides medical and biological applications [6]. Hine [7] showed that a constant value of atomic number is not suitable for photon interaction across the entire energy region. The parameter denoting the atomic number of a sample with different chemical constituents is the effective atomic number and it can be obtained by different ways such as logarithmic

interpolation, power law, auto-Z_{eff} and direct method [8–11]. Z_{eff} is not constant and it varies with energy depending on dominant interaction processes. In low-energy region ($E < 0.05$ MeV) photoelectric absorption is dominant and proportional to Z^4 of an absorber. Dominance of Compton scattering and pair production in intermediate (0.05 MeV $< E <$ 1.02 MeV) and high-energy region ($E > 1.02$ MeV) is proportional to Z and Z^2 respectively.

Several researchers have investigated γ-photon interaction on different types of materials. The electron density (N_{eff}) and effective atomic number (Z_{eff}) were found to be higher at low energy for carbohydrates and fatty acids as studied by Manohara *et al* [12]. Manjunathaguru and Umesh [13] computed the electron density (N_{eff}) of amino acids using the new matrix method. Recently, mass attenuation coefficients for a few medicinal plants were measured by Morabad and Kerur [14]. Gamma-ray transmission studies on C-, H-, N- and O-based biological molecules have been carried out with a narrow-beam good geometry set-up, and it is reported that the mass attenuation coefficient decreases with increase in energy [15–18]. The attenuations of high-energy photons by biologically important systems, tissues and materials of dosimetric interest have been carried out by a few investigators [19–28].

A fatty acid is an acid consisting of a saturated or an unsaturated hydrocarbon chain with a terminal carboxyl group. Fatty acids do not exist in a free state, and are always found combined with triglycerides. Fatty acids are necessary for the growth and functioning of living cells and their deficiency may cause critical disease or abnormality. No experimental data on atomic and electronic scattering cross-sections are reported in the literature for the present samples, which are most convenient for the computation of Z_{eff} and other parameters. This promoted a systematic and comprehensive investigation of fatty acids in the energy range 122–1330 keV. In the present work, the mass attenuation coefficient (μ_{m}), effective atomic number (Z_{eff}), effective electron density (N_{eff}), atomic cross-section (σ_{t}) and electronic cross-section (σ_{e}) of fatty acids have been determined experimentally in the energy range 122–1330 keV. The experimental results were compared with the theoretical values.

2. Theory

The theoretical formulation for the calculation of mass attenuation coefficient (μ_{m}) and other related parameters are reviewed below. When a monochromatic beam of γ-ray is collimated on a sample, photons are attenuated by the sample due to absorption and scattering. The transmitted beam of photons is represented by

$$I = I_0 \mathrm{e}^{-\mu t}, \tag{1}$$

where I_0 and I are respectively the initial and final intensities of the interacting photons. μ (cm^{-1}) is the linear attenuation coefficient of the sample that decreases exponentially and t (cm) is the thickness of the material. The linear attenuation coefficient (μ) of the materials from eq. (1) is expressed as

$$\mu = \frac{1}{t} \ln\left(\frac{I_0}{I}\right), \tag{2}$$

where $\ln(I_0/I)$ is the absorbance which depends on the density, Z and thickness of the sample. By introducing the density of the material in eq. (2), the mass attenuation coefficients for a sample is given by

$$\mu_{\text{m}} = \frac{\mu}{\rho}(\text{cm}^2\ \text{g}^{-1}) = \frac{1}{\rho t} \ln\left(\frac{I_0}{I}\right), \tag{3}$$

where the density (ρ) is expressed in g/cm^3.

The fatty acids are composed of the elements C, H and O in different proportions, and their constituent elements participate in the interaction process and is additive. The mass attenuation coefficient (μ_{m}) of such a compound is represented by the sum of the weighted fractions of the individual atoms of the element according to the mixture rule [5]. Then, the mass attenuation coefficient (μ_{m}) for the selected compound can be written as

$$\mu_{\text{m}} = \sum_i W_i (\mu_{\text{m}})_i, \tag{4}$$

where W_i and $(\mu_{\text{m}})_i$ are the weight fraction and mass attenuation coefficient for the ith constituent element, respectively. The weight fraction (W_i) for the compound is the ratio of atomic weight of the individual elements and total atomic weight of the compound and is represented by

$$W_i = \frac{n_i A_i}{\sum_j n_i A_j}, \tag{5}$$

where A_i and n_i are the atomic weight of the ith constituent element and number of formula units respectively. The total photon interaction cross-section (σ) contributed by various partial interaction processes is expressed as

$$\sigma = \sigma_{\text{pho}} + \sigma_{\text{incoh}} + \sigma_{\text{coh}} + \sigma_{\text{pair}} + \sigma_{\text{tri}} + \sigma_{\text{ph.n.}}, \tag{6}$$

where σ_{pho} is the atomic photoelectric absorption cross-section that occurred in the energy region below 0.01 MeV and σ_{incoh} is the Compton scattering (incoherent) dominant at intermediate energy region, 0.05 MeV $< E <$ 5 MeV. The scattering process which occurred in the high-energy region, above 1.02 MeV, such as σ_{pair} and σ_{tri}, are pair production in the field of nucleus and electron. $\sigma_{\text{ph.n}}$ is the photonuclear scattering cross-section. The molecular scattering cross-section ($\sigma_{\text{t,m}}$) determined using the mass attenuation coefficient (μ_{m}) is given by

$$\sigma_{\text{t,m}} = \mu_{\text{m}}(M/N_{\text{A}}), \tag{7}$$

where $M = \sum_i n_i A_i$ is the molecular weight, N_{A} is the Avogadro's number, n_i is the number of atoms in the molecule and A_i is the atomic weight of the ith element in a molecule. Similarly, the atomic cross-section (σ_{t}) is represented by

$$\sigma_{\text{t}} = \frac{1}{N_{\text{A}}} \sum_i f_i A_i (\mu_{\text{m}})_i. \tag{8}$$

The electronic cross-section (σ_{e}) is the ratio of the atomic cross-section and effective atomic number (Z_{eff}) and is denoted by the following relation:

$$(\sigma_{\text{e}}) = \frac{1}{N_{\text{A}}} \sum_i \frac{f_i A_i}{Z_i} (\mu_{\text{m}})_i = \frac{\sigma_{\text{t}}}{Z_{\text{eff}}}, \tag{9}$$

where Z_i is the atomic number of the ith constituent element. Rearranging eq. (9) yields Z_{eff} represented by

$$Z_{\text{eff}} = \frac{\sigma_{\text{t}}}{\sigma_{\text{e}}}. \tag{10}$$

Equation (10) is closely related to the effective electron density (N_{eff}) (number of electrons per unit mass). Now, mass attenuation coefficient (μ_{m}) and electronic cross-section (σ_{e}) make it possible to calculate N_{eff} per unit volume of the sample as

$$N_{\text{eff}} = \frac{\mu_{\text{m}}}{\sigma_{\text{e}}} = \frac{N_{\text{A}}}{M} Z_{\text{eff}} \sum_i n_i, \tag{11}$$

where μ_{m} and M/n are the mass attenuation coefficient and average atomic weight respectively, $\sum_i n_i = n$ is the total number of atoms. The theoretical mass attenuation coefficient values were derived from XCOM program based on mixture rule [29].

3. Experimental details

The fatty acids, viz. undecylic acid ($C_{11}H_{22}O_2$), lauric acid ($C_{12}H_{24}O_2$), tridecylic acid ($C_{13}H_{26}O_2$), myristic acid ($C_{14}H_{28}O_2$), pentadecylic acid ($C_{15}H_{30}O_2$) and palmitic acid ($C_{16}H_{32}O_2$) were weighed using a sensitive digital balance to the third decimal place. Radioactive sources such as ^{57}Co (250 kBq), ^{133}Ba (86 kBq), ^{137}Cs (97 kBq), ^{60}Co (134 kBq) and ^{22}Na (73kBq) used for transmission experiments were obtained from Bhabha Atomic Research Centre, Mumbai. The transmission experiment was carried out using a $3'' \times 3''$ NaI(Tl) scintillation detector having 8.2% resolution at 662 keV. The detector and γ-ray source were shielded well using lead. A plastic container was used as a sample holder, and attenuation of the photon by the unfilled container was found negligible. The detector spectrometer was calibrated in the energies 122, 356, 511, 662, 1170, 1275 and 1330 keV using the radioactive sources ^{57}Co, ^{133}Ba, ^{137}Cs, ^{60}Co and ^{22}Na, then the spectra were recorded with and without fatty acids. The transmitted photons were amplified and analysed by an 8K multichannel analyser. The distance (30 cm $\leq d \leq$ 50 cm) between the detector and the sample was adjusted so that the maximum angle of scattering was within 30 min. An optimum thickness ($2 < \ln(I_0/I) < 4$) of the samples was selected to minimize multiple scattering. Details of the experimental arrangement have been discussed earlier by Pawar and Bichile [16].

4. Results and discussion

The mean atomic numbers $\langle Z \rangle$ are calculated using the chemical formula for fatty acids and listed in table 1. The experimentally measured attenuation cross-sections of the fatty acids, undecylic acid ($C_{11}H_{22}O_2$), lauric acid ($C_{12}H_{24}O_2$), tridecylic acid ($C_{13}H_{26}O_2$), myristic acid ($C_{14}H_{28}O_2$), pentadecylic acid ($C_{15}H_{30}O_2$) and palmitic acid ($C_{16}H_{32}O_2$) in the energy range 122–1330 keV carried out by employing the NaI(Tl) detector with a well-collimated narrow beam good geometry set-up, are shown in tables 2, 3, 4, 5 and 6 along with theoretical results. The experimentally measured mass

Table 1. The mean atomic numbers calculated from the chemical formula for fatty acids.

Fatty acids	Molar mass (g/mol)	Chemical formula	Mean atomic number, $\langle Z \rangle$
Undecylic acid	186.29	$C_{11}H_{22}O_2$	2.97
Lauric acid	200.32	$C_{12}H_{24}O_2$	2.95
Tridecylic acid	214.35	$C_{13}H_{26}O_2$	2.93
Myristic acid	228.37	$C_{14}H_{28}O_2$	2.91
Pentadecylic acid	242.40	$C_{15}H_{30}O_2$	2.89
Palmitic acid	256.43	$C_{16}H_{32}O_2$	2.88

Table 2. Mass attenuation coefficient (μ_m) (cm^2/g) of fatty acids.

	122 keV		356 keV		511 keV		662 keV		1170 keV		1275 keV		1330 keV	
Fatty acids	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo
Undecylic acid	0.160	0.159	0.110	0.111	0.094	0.095	0.086	0.085	0.065	0.066	0.060	0.161	0.060	0.060
Lauric acid	0.169	0.170	0.112	0.111	0.093	0.094	0.087	0.086	0.066	0.065	0.062	0.061	0.061	0.060
Tridecylic acid	0.171	0.170	0.114	0.113	0.097	0.098	0.085	0.086	0.067	0.068	0.060	0.061	0.060	0.060
Myristic acid	0.160	0.161	0.114	0.113	0.096	0.095	0.085	0.086	0.067	0.066	0.062	0.061	0.060	0.060
Pentadecylic acid	0.162	0.161	0.112	0.113	0.095	0.096	0.086	0.085	0.065	0.066	0.060	0.061	0.060	0.060
Palmitic acid	0.163	0.162	0.113	0.112	0.096	0.097	0.087	0.086	0.066	0.065	0.060	0.061	0.061	0.060

Table 3. Atomic cross-sections (σ_t) (barn/molecule) of fatty acids.

	122 keV		356 keV		511 keV		662 keV		1170 keV		1275 keV		1330 keV	
Fatty acids	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.
Undecylic acid	49.473	49.163	34.012	34.321	29.065	29.374	26.592	26.282	20.098	20.407	18.552	18.861	18.552	18.552
Lauric acid	56.190	56.523	37.238	36.906	30.921	31.254	28.926	28.594	21.944	21.612	20.614	20.282	20.282	19.950
Tridecylic acid	60.836	60.480	40.557	40.202	34.509	34.865	30.240	30.596	23.836	24.162	21.350	21.702	21.350	21.346
Myristic acid	60.647	61.027	43.211	42.832	36.389	36.010	32.219	32.598	25.396	25.017	23.501	23.122	22.743	22.743
Pentadecylic acid	65.177	64.775	45.061	45.463	38.221	38.624	34.600	34.198	26.151	26.554	24.140	24.542	24.140	24.140
Palmitic acid	69.374	68.949	48.094	47.668	40.859	41.284	37.028	36.730	28.090	27.665	25.537	25.962	25.962	25.536

Table 4. Electronic cross-sections (σ_e) (barn/molecule) of fatty acids.

	122 keV		356 keV		511 keV		662 keV		1170 keV		1275 keV		1330 keV	
Fatty acids	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.
Undecylic acid	7.949	17.843	12.173	12.279	10.352	10.458	9.431	9.325	7.074	7.185	6.633	6.527	6.521	6.523
Lauric acid	20.619	20.733	13.338	13.453	11.123	11.239	10.361	10.245	7.798	7.683	7.317	7.201	7.195	7.079
Tridecylic acid	22.513	22.389	14.781	14.657	12.521	12.646	10.932	11.057	8.547	8.672	7.645	7.769	7.637	7.637
Myristic acid	22.647	22.780	15.873	15.740	13.297	13.163	11.737	11.871	9.168	9.035	8.473	8.340	8.197	8.198
Pentadecylic acid	24.483	24.341	16.671	16.814	14.065	14.208	12.674	12.531	9.505	9.648	8.763	8.906	8.754	8.754
Palmitic acid	26.222	26.071	17.886	17.734	15.112	15.275	13.641	13.537	10.260	10.108	9.322	9.474	9.464	9.312

Table 5. Effective atomic number (Z_{eff}) of fatty acids.

	122 keV		356 keV		511 keV		662 keV		1170 keV		1275 keV		1330 keV	
Fatty acids	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.
Undecylic acid	2.756	2.755	2.794	2.795	2.808	2.809	2.820	2.819	2.841	2.840	2.842	2.843	2.844	2.845
Lauric acid	2.725	2.726	2.768	2.767	2.780	2.781	2.792	2.791	2.814	2.813	2.817	2.816	2.819	2.818
Tridecylic acid	2.702	2.701	2.744	2.743	2.756	2.757	2.766	2.767	2.789	2.790	2.792	2.793	2.795	2.795
Myristic acid	2.768	2.680	2.722	2.721	2.737	2.736	2.745	2.746	2.770	2.769	2.773	2.772	2.774	2.774
Pentadecylic acid	2.662	2.661	2.703	2.704	2.718	2.719	2.730	2.729	2.751	2.752	2.755	2.7556	2.758	2.758
Palmitic acid	2.646	2.645	2.689	2.688	2.704	2.703	2.714	2.713	2.738	2.737	2.739	2.740	2.743	2.742

Table 6. Effective electron densities (N_{eff}) (10^{24}) of fatty acids.

	122 keV		356 keV		511 keV		662 keV		1170 keV		1275 keV		1330 keV	
Fatty acids	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo.	Exp.	Theo
Undecylic acid	0.3120	0.3119	0.3163	0.3164	0.3178	0.3179	0.3192	0.3190	0.3216	0.3215	0.3217	0.3219	0.3219	0.3220
Lauric acid	0.3115	0.3116	0.3164	0.3162	0.3177	0.3179	0.3191	0.3190	0.3216	0.3215	0.3220	0.3219	0.3222	0.3221
Tridecylic acid	0.3114	0.3113	0.3162	0.3161	0.3176	0.3177	0.3188	0.3189	0.3214	0.3215	0.3219	0.3219	0.3221	0.3221
Myristic acid	0.3110	0.3111	0.3161	0.3160	0.3178	0.3176	0.3187	0.3189	0.3216	0.3215	0.3220	0.3219	0.3222	0.3221
Pentadecylic acid	0.3110	0.3109	0.3158	0.3159	0.3175	0.3156	0.3189	0.3188	0.3214	0.3215	0.3218	0.3219	0.3221	0.3221
Palmitic acid	0.3108	0.3107	0.3159	0.3158	0.3176	0.3175	0.3189	0.3188	0.3215	0.3215	0.3218	0.3219	0.3223	0.3222

attenuation coefficients (μ_m) are tabulated in table 2 for all samples. This is the most widely used physical quantity for therapy computations and applicable in health physics, radiation shielding and nuclear medicine. Figure 1 depicts variations of μ_m with photon energy for undecylic acid ($C_{11}H_{22}O_2$), and it is observed that μ_m decreases with increasing photon energy and finally the value stabilizes due to the dominance of Compton scattering and pair production in the corresponding energy region. For the present energy range, Compton scattering is the main dominating interaction process which occurred up to 150 keV having valuable applications in diagnostic imaging. It is clearly seen from table 2 and figure 1, that μ_m depends upon the energy of the interacting photons and effective atomic number of the fatty acids. Variations in the measured values of σ_t and σ_e are similar in nature and are tabulated in tables 3 and 4, respectively. Scattering cross-section data, which reveal structural information, are very important in biological systems. The atomic and electronic cross-sections as a function of energy are plotted in figures 2 and 3 for undecylic acid ($C_{11}H_{22}O_2$) and it is seen that σ_t and σ_e decrease with the interacting photon energy. Z_{eff} as a function of energy is displayed in figure 4. It can be clearly seen from table 5 that the behaviour of Z_{eff} is similar for all samples. As all fatty acids have the same constituent elements, and variation in Z_{eff} is very little with photon energy, Z_{eff} tends to a constant value. The known values of effective atomic number (Z_{eff}) can be utilized

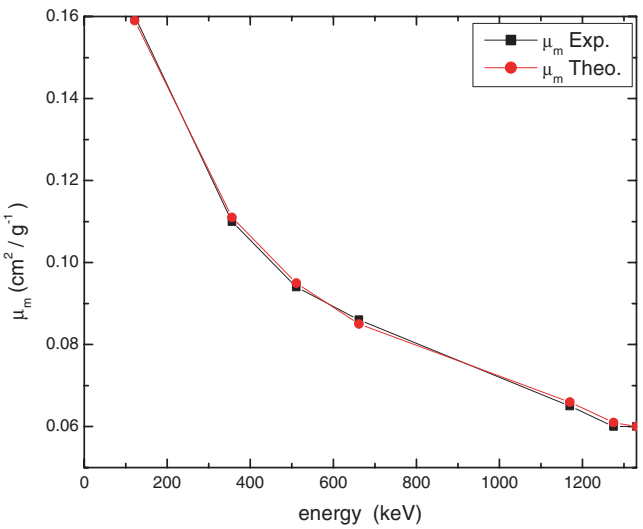

Figure 1. The typical plot of μ_m vs. energy E for undecylic acid ($C_{11}H_{22}O_2$).

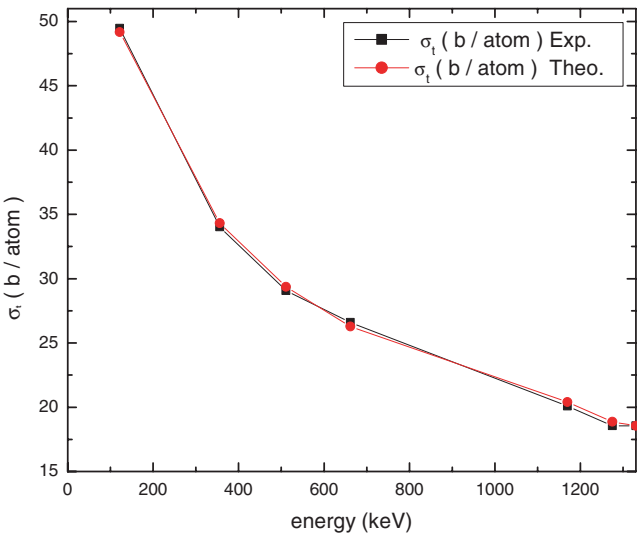

Figure 2. The typical plots of σ_t vs. E for undecylic acid ($C_{11}H_{22}O_2$).

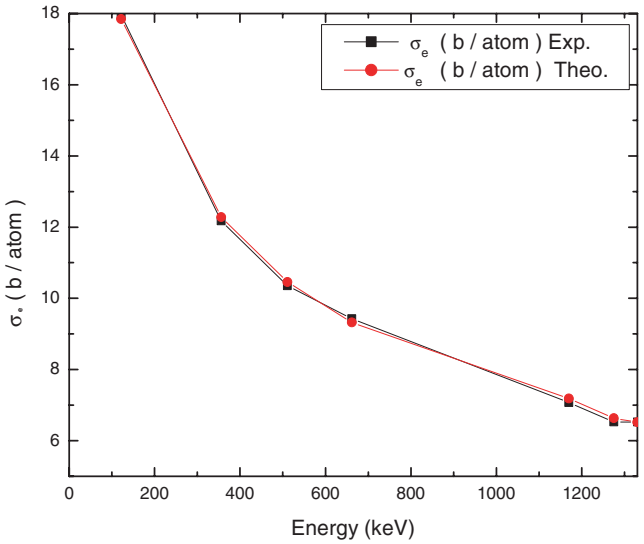

Figure 3. The typical plots of σ_e vs. E for undecylic acid ($C_{11}H_{22}O_2$).

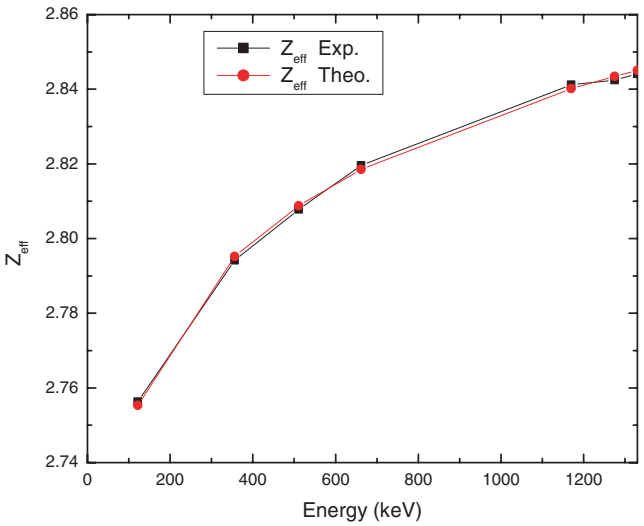

Figure 4. The typical plots of Z_{eff} vs. E for undecylic acid ($C_{11}H_{22}O_2$).

to calculate the absorbed dose and build-up factor for dose and radiation therapy calculation. For the present samples, Z_{eff} values in the energy range 122–1330 keV are found to be closely related to the average atomic number, as the Compton scattering cross-section is proportional to the atomic number of an absorber. The values of N_{eff} vary very little with energy as shown in figure 5. The mass attenuation coefficient (μ_m) and the total electronic cross-section (σ_e) values were used to calculate N_{eff} and the same are listed in table 6.

The overall estimated error observed in the measurement of cross-section is less than 2%. The error in the

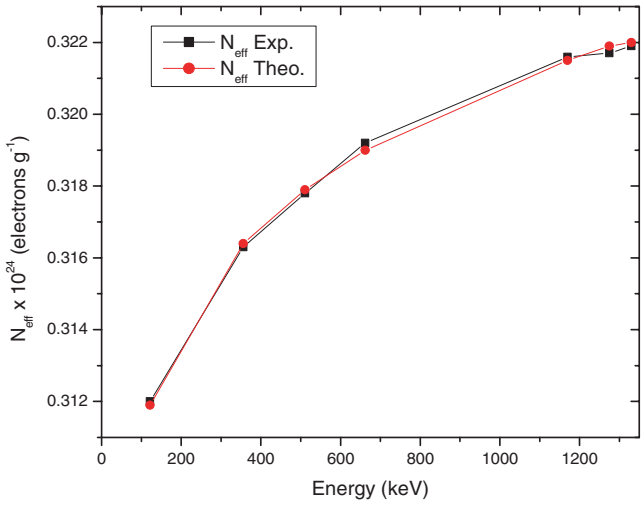

Figure 5. The typical variation of effective electron density N_{eff} vs. photon energy for undecylic acid ($C_{11}H_{22}O_2$).

measurement is the sum of uncertainties in thickness (<0.6%), impurity and non-uniformity of a sample. The photon build-up, multiple scattering and pulse pile-up effects were reduced to minimum by choosing optimum thickness ($\mu t < 4$) of the sample and optimum count rate and counting time of a detector with a good resolution. The given samples were in 99.9% pure form with the intention that impurity corrections were not applied to the obtained results. The error occurred due to the non-uniformity of the sample was less than 0.05%. The transmission experiment was performed and repeated for each sample with periods of 200 s–800 s in order to minimize statistical uncertainty (<0.5%). A very small deviation in count was observed after every repetition, confirming the sensitivity of the instrument. For the present energy range, small-angle scattering corrections were not applied. However, photons transmitted through the sample were collimated and detected by the NaI(Tl) scintillation detector with a good energy resolution.

5. Conclusion

The mass attenuation coefficients (μ_m) of fatty acids, viz., undecylic acid ($C_{11}H_{22}O_2$), lauric acid ($C_{12}H_{24}O_2$), tridecylic acid ($C_{13}H_{26}O_2$), myristic acid ($C_{14}H_{28}O_2$), pentadecylic acid ($C_{15}H_{30}O_2$) and palmitic acid ($C_{16}H_{32}O_2$) have been calculated at energies 122, 360, 511, 662, 1170, 1275 and 1330 keV, respectively. These values were used to calculate N_{eff}, Z_{eff}, σ_t and σ_e and are almost constant above 1.12 MeV. The electron densities for the presently studied fatty acids are found to be in the range of (0.3108–0.3223)*10^{24}.

The present results of fatty acids in the energy range up to 1330 keV should be useful in food preservation and packing, besides in nuclear medicine, radiation therapy and diagnosis applications. Data on interaction of photons of energy (below 1500 keV) with biological compounds are used in radiation therapy, especially for dose calculations. For food preservation and packing, radiation is used as it is necessary to understand the interaction of radiation with biological compounds.

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