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Determination of attenuation parameters and energy absorption build-up factor of amine group materials

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ABSTRACT

Keywords: Mass attenuation coefficient (μ_m) Effective atomic number (Z_{eff}) Effective electron density (N_{eff}) G-P fitting method Energy absorption build up factor (EABF) We have computed radiological parameters of some C- H- N- O based amine group bio material in the energy range 122–1330 keV with the gamma ray count by narrow beam geometry. The NaI(Tl) detector with 8 K multichannel analyser was used having resolution 6.8% at 663 keV. The energy absorption buildup factor (EABF) was determined by using Geometric Progression (G-P) fitting method up to penetration depth of 40 mfp at energy 0.015–15 MeV. The NIST XCOM data were compared with the experimental value and we observed (3–5%) difference. The comparative study of effective atomic number and effective electron density in the energy range 122–1330 keV using Gaussian fit for accuracy were performed. The amino acid has the highest EABF value at 0.1 MeV and the variation in EABF with penetration depth up to 1–40 mean free path (mfp). The calculated radiological data of biological material are applicable in medical physics and dosimetry.

1. Introduction

Mass attenuation coefficient (μ m), effective atomic number (Z_{eff}), effective electron density (N_{eff}), molar extinction coefficient are basic parameters to find the penetration and energy deposition of gamma radiation ([Gounhalli et al., 2012;](#page-7-0) [Manjunatha et al., 2016;](#page-7-1) [El-Khayatt](#page-7-2) [et al., 2014](#page-7-2)). Gamma radiation is used in diverse fields such as agriculture [\(Pires et al., 2016\)](#page-7-3), industry, medical [\(Manohara et al., 2007](#page-7-4)), radiation dosimetry [\(Gowda et al., 2004\)](#page-7-5), diagnosis, shielding [\(Otto](#page-7-6) [et al., 2012](#page-7-6); [Biswas et al., 2016](#page-7-7)), gamma ray fluorescence ([Ekinci et al.,](#page-7-8) [2007\)](#page-7-8), drug delivery [\(Gounhalli et al., 2012\)](#page-7-0), radiation biophysics, science and technology [\(McCullough et al., 1975](#page-7-9)) etc. The NaI(Tl) detector is a spectrometric system to show the fine spectra at room temperature and its economic device has good efficiency ([Medhat et al.,](#page-7-10) [2014\)](#page-7-10). The ratio of mass energy absorption coefficient and the back scattered factor for diagnosis for mono-energetics database photon with lower energy ([Benmakhlouf et al., 2011\)](#page-7-11). The mass attenuation coefficient parameter is a chemical composition dependent parameter for dosimetric and tissue substitute material ([El-Khayatt et al., 2014\)](#page-7-2) and also depends on the physical as well as chemical environment of the nonessential amino acids (Bursalıoğ[lu et al., 2014\)](#page-7-12). The uncertainties in the calculation of the mass attenuation coefficient are dependent on the process of calculation and the radionuclide of gamma ray spectra ([Andreo et al., 2012\)](#page-7-13). The other parameter atomic, molecular and electronic effective cross sections are playing an important role in the distribution of photon flux for any object (Bursalıoğ[lu et al., 2014](#page-7-12)).

Average Molar extinction coefficient value of the biological material is less than the theoretical value ([Pace et al., 1995](#page-7-14)). The atomic number of composite materials is depending on the energy; a number cannot show atomic number of the material in entire energy region i.e. effective atomic number ([Gowda et al., 2004, 2005;](#page-7-5) [Hine et al., 1952](#page-7-15)). The Z_{eff} of particular energy of body tissue components depends on different interaction processes and atomic number. [Degrelle et al. \(2016\)](#page-7-16) Explaining two methods to calculate mass attenuation coefficient using Monte Carlo simulation and discussed about the self-absorption phenomena are only dependent on the coefficient and not on the density of the material. Scattering does not affect at large scale on the organs and the values of Zeff determined by NEPEA are in good agreement with Compton process ([Torikoshi et al., 2007\)](#page-7-17). A new method to calculate Z_{eff} for the total cross section in Compton scattering process at the nuclear energy 1464 keV has been developed ([Kaliman et al., 2007](#page-7-18)). Z_{eff} of amino acids depends on their side chain and the behaviour as Z_{eff} decreases, the hydrophobicity increases of the unionized amine group material ([Gowda et al., 2005\)](#page-7-19).

The gamma-ray buildup factors are most used in the shielding calculation for gamma-ray sources ([Singh et al., 2013\)](#page-7-20). Gamma ray buildup factor is important in the distribution of photon flux for the calculation of radiation dose of biological molecules. There are two types of buildup factors: (a) Energy absorption buildup factor (b) exposure buildup factor. Energy absorption buildup factor in which quantity of interest is the absorbed or deposited energy in the interacting material and the detector response function is that of absorption

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Fig. 1. The schematic view of narrow beam geometry of NaI(Tl) Detector.

in the interacting material. Different methods were used by various research groups to compute the buildup factors G. P. fitting method by [Harima et al. \(1986\)](#page-7-21), invariant embedding method by [Sakamaoto and](#page-7-22) [Tanaka \(1988\)](#page-7-22) and [Shimizu \(2002\),](#page-7-23) iterative method by [Suteau and](#page-7-24) [Chiron \(2005\)](#page-7-24) and Monte Carlo method by [Sardari et al. \(2009\).](#page-7-25)

The amino acids are a basic building block of living organism. All living things basic constituents are amino acids. e.g. DNA and RNA (also made up of amino acids). The human body uses 20 different amino acids for building peptides and proteins. The amino acids are classified into two types: essential amino acids and nonessential amino acids. Amino acids are polar in nature [except Glycine (CH_2NH_3COOH)]. There are two types one is R/D amino acid and S/L Amino acids. D- (Dextro) rotatory PPL (Plane polarized light) in a right hand direction called as clockwise direction and L-(leovo) rotatory PPL in a left hand direction called as anticlockwise direction. Due to polar nature amino acid acts as solvent, it solvalize the reaction. It's an organic solvent naturally occurred. Amino acid having intra hydrogen bonding called Zwiter ion which is neutral species.

The objective of the present work is to show accurate variation of the experimentally observed radiological parameters 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 amino acids in the energy range 122–1330 keV for the gamma radiation using narrow beam geometry. Theoretically energy absorption buildup factor in the 0.015–15 MeV energy range up to penetration depth 40 mfp of amine group biological material using geometric progression fitting method. Also studied the effect of the penetration depth on EABF at different energy. This study gives basic knowledge about calculation of shielding properties of biological materials. It should be noted that the necessity of biological materials like amino groups to control the radiation level for the protection aspects of radiology.

2. Experimental and calculation method

The radioactive sources 57 Co, 133 Ba, 137 Cs, 54 Mn, 60 Co and 22 Na were used to generate gamma rays for the experiment. The gamma ray energies emitted by these sources are 122, 360, 511, 662, 840, 1170, 1275 and 1330 keV respectively. The gamma rays emitted by these radioactive sources were collimated and detected by the NaI(Tl) scintillation detector. The sources are perpendicular to the surface of the material. The selected gamma ray spectroscopic system was the narrow beam geometry shown in [Fig. 1.](#page-1-0) As the high Z of iodine in NaI may have good efficiency ([Kaçal et al., 2012](#page-7-26)). The signals from the detector $(2'' \times 2'')$ NaI(Tl) crystal having energy resolution of 8.2% at 662 keV gamma rays from the decay of Cs^{137} after suitable amplification (according to full width at half maxima FWHM) was recorded in EG & G ORTEC 13-bit plug-in-card coupled to a PC/AT. The stability and reproducibility of the arrangement were checked before and after each set of runs in the usual manner. The system shows fine acquires gamma ray spectra to provide accurate information at below room temperature (20 °C to 23 °C). All amine group material (Aspartic acid, Monosodium salt monohydrates, D-Arginine monohydrochloride, D-Asparagine Monohydrates, p-Glutamic acid, DL-Arginine, DL-arginine monohydrochloride monohydrates) had good purity (99%). The sample thickness was selected in order to satisfy the following ideal condition as far as possible [\(Creagh et al., 1987](#page-7-27)). The pellet of amine group material was prepared by using a KBr press machine (up to pressure 10 t) with 0.13 g/cm² of uniform thicknesses and confined in a cylindrical plastic container having the same diameter as that of sample pellets. The diameters of the samples were determined with the help of a travelling microscope. Weights of pallet were measured by using digital balance having 0.001 mg accuracy. We measured value of I_o (unattenuated photon intensity) with empty plastic container and I (attenuated photon intensity) with sample at narrow beam geometry set up. The mass attenuation coefficient μ_m for all amine group material were calculated using Eq. [\(3\)](#page-2-0) and theoretically observed by NIST XCOM database at selected incident photon energy. Proper adjustment of the distance between the detector and source (30 cm \leq d \leq 50 cm), the maximum angle of scattering was below 30 min. In the multichannel analyser used in the present study, there was a built-in provision for dead time correction.

2.1. Mass attenuation coefficient

The measurement of mass attenuation coefficient of the amino acids was performed for homogeneous medium by using Lambert Beer exponential attenuation law,

$$
I = I_0 e^{\mu x} \tag{1}
$$

where I_0 and I are the unattenuated and attenuated photon intensity respectively, μ is the linear attenuation coefficient; X is the thickness of the sample. The ratio of linear attenuation coefficients and density of material called as mass attenuation coefficients (??/??).

2.2. Molar extinction coefficient

The material or solvent absorb light per unit mass density called as

|--|--|

The mean atomic numbers calculated from the chemical formula for the investigated amino acids.

Table 2

Mass attenuation coefficient (cm²/g) for the investigated amino acids.

Fig. 2. Variation of $\upmu_{\rm m}$ vs energy for DL-Arginine.

molar extinction coefficient or molar absorptivity shown below,

 $\mathcal{E} = 0.4343 \text{ N}_{A} \sigma_{t}$ (2)

 N_A is the Avogadro constant and σ_t is the total attenuation cross section

2.3. Total atomic cross section

Firstly, we calculate the total attenuation cross section:

$$
\sigma_t = \frac{1}{N_A} \sum f_i A_i(\mu_m) \tag{3}
$$

 N_A is the Avogadro constant, μ_m is the mass attenuation coefficient and A_i is the molar mass of the sample. $\Sigma f_i = 1$ (f_i is the mole fraction) ([More et al., 2016](#page-7-28))

$$
\sigma_a = \frac{\sigma_t}{\sum n_i} \tag{4}
$$

 Σ n_i is the total number of the ith constituent

Table 3
Total at

Total attenuation cross-sections, σ_τ 10²³(barn/atom) of the amino acids.

2.4. Electronic cross section

$$
\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} (\mu_m)_i = \frac{\sigma_t}{\sum Z_{\text{eff}}}
$$
(5)

Electronic cross section is the ratio of total attenuation cross section and effective atomic number shows in above written formula.

2.5. The effective atomic number (Z_{eff})

Compton scattering interaction process of the composite material depends on effective atomic number ([Gowda et al., 2005](#page-7-19)), which is discussed by [Manohara et al. \(2008\).](#page-7-29)

$$
Z_{\text{eff}} = \frac{\sigma_t}{\sigma_e} \tag{6}
$$

2.6. Effective electron density

Effective electron density shows that the number of electron per unit mass

$$
N_{\text{eff}} = \left(\frac{N_A}{A_{\text{eff}}}\right)^* Z_{\text{eff}} \tag{7}
$$

Aeff is effective atomic mass also known as the ratio of atomic weight and total number of atom

3. The computation of energy absorption buildup factor

The computation of EABF using G-P Fitting method and equivalence atomic number of selected amino acids. There are three steps

- 1) Calculate equivalence atomic number (Z_{eq}) .
- 2) Computation of geometric progression (G-P) parameters.
- 3) Calculating the energy absorption buildup factor.

1) Calculate equivalence atomic number (Z_{eq}) :

Table 4

Molar extinction coefficients, ε (cm²/mole) of the investigated amino acids.

Table 5

Total atomic cross-sections, σ_a 10²⁴(barn/atom) of the amino acids.

Table 6

Electronic cross-sections, σ_e 10²⁵(barn/atom) of the investigated amino acids.

Fig. 3. Variation of σ_t vs energy for DL-Arginine.

The Z_{eq} depends on the chemical composition of materials. The different energy shows the different interaction processes such as photoelectric, Compton or pair production. The Z_{eq} defined by [Kurudirek and Özdemir \(2011\)](#page-7-30) for computation of equivalent atomic number, the ratio of Compton partial attenuation coefficient $(\mu_{\rm m})_{\rm comp}$ and total attenuation coefficient $(\mu_{\rm m})_{\rm total}$ interacting material have been interpolated within the corresponding ratios $(\mu_{\text{Comp}}/\mu_{\text{total}})$ database of the elements at the same energy (0.015–15 MeV). The total mass attenuation coefficient $(\mu_{\rm m})_{\rm comp}$

and partial Compton attenuation coefficient (μ_m) total were calculated by using NIST- XCOM data base.

$$
Z_{eq} = \frac{Z_1(logR_2 - logR) + Z_2(logR - logR_1)}{logR_2 - logR_1}
$$
(8)

Where R is the ratio of selected biological materials at given energy. The Z_1 and Z_2 are the elemental atomic number corresponding to the ratio R_1 and R_2 respectively.

2) Computation of geometric progression (G-P) parameters

The buildup factor data for 23 elements, one compound, two mixtures (air and water) and concrete at energies in the range 0.015–15 MeV up to penetration depths of 40 mfp using the G-P Method Provided by American National Standards [\(ANSI/ANS-](#page-7-31)[6.4.3, 1991](#page-7-31)). Using the interpolation formula, five G.P. fitting parameters (b, c, a, X_k and d) for selected samples were computed at the different incident photon energies using equivalent atomic number (Zeq), in the chosen energy range (0.015.15.0 MeV) up to penetration depth of 40 mfp. The formula used for the purpose of interpolation is

$$
C = \frac{C_1(\log Z_2 - \log Z_{eq}) + C_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1}
$$
(9)

where C_1 and C_2 are the values of the coefficients of G-P fitting

Fig. 4. Variation of σ _a vs energy for DL-Arginine.

Fig. 5. Variation of ε vs energy for DL-Arginine.

Fig. 6. Variation σ_e vs energy for DL-Arginine.

Table 7 Effective atomic number, Z_{eff} of the investigated amino acids.

parameters corresponding to the atomic numbers Z_1 and Z_2 , respectively at a given energy and Z_{eq} is the equivalent atomic number of the given material.

4. Computation of energy absorption buildup factor

Firstly, computed G. P. fitting parameters were then used to compute the energy absorption and exposure buildup factors for the selected samples at some standard incident photon energies up to a penetration depth of 40 mean free paths of shielding thickness as given by following equations, with the help of G.P. fitting formula,

$$
B(E, X) = 1 + \frac{b-1}{K-1}(K_x - 1) At K \neq 1
$$
\n(10)

$$
B(E, X) = 1 + (b - 1) At K = 1
$$
\n(11)

$$
K(E, x) = cx^{a} + d \frac{\tanh(\frac{x}{x_{k}} - 2) - \tanh(-2)}{1 - \tanh(-2)}
$$
(12)

Where parameters b and K are corresponding to a buildup factor at 1 mfp and a multiplication factor of dose through 1 mfp photon penetration, respectively. Parameter K is obtained by for X using parameters b, c, a, d and X_k .

5. Result and discussion

The photon interaction parameters like mass attenuation coefficient, total atomic cross section, molar extinction coefficient, total electronic cross section, effective atomic number, effective electron density of the some amine group biological material such as Aspartic acid, Monosodium salt monohydrates (A), D-Arginine monohydrochloride (B), D-Asparagine mono Hydrates (C), D-Glutamic acid(D), DL-Arginine (E), DL-arginine monohydrochloride monohydrates(F) were calculated in the energy region 122–1330 keV. The application of selected energy region is in the medical diagnosis. [Table 1](#page-1-1) shows the chemical and physical parameter of the sample calculated by standard formulae. [Table 2](#page-2-1) shows that the mass attenuation coefficient of the biological material shows the variation as compared to the theoretical value. Theoretical data represented by the NIST XCOM program and experimental data with narrow beam photon interaction with the material have slight variation. The variation in the theoretical and experimental value of the mass attenuation coefficient is dependent on chemical composition and thickness of the sample. [Fig. 2](#page-2-2) shows for a single selected amino acid for checking the behaviour of the mass attenuation coefficient with energy. This shows that the energy is increasing, the mass attenuation coefficient of the sample is decreasing. The CT scanning is related to the interaction process coherent (Rayleigh-Jeans scattering), photoelectric and incoherent scattering (Compton scattering). The Compton scattering is dominated for biological materials by E. c. McCullough similarly our result shows the same. The [Tables 3, 5](#page-2-3) [and 6](#page-2-3) shows the total attenuation cross section, total atomic cross section, and electronic cross section. The earlier studies by ([Bursal](#page-7-12)ıoğlu

Fig. 7. Variation of Z_{eff} energy for DL-Arginine.

[et al., 2014\)](#page-7-12) for this parameter, comparably both shows equal behaviour of result and the value of amino acid decreases with increasing photon energy graphically shown in [Figs. 3, 4 and 6.](#page-3-0) Molar extinction coefficients were tabulated in [Table 4](#page-3-1) and graphically represented in [Fig. 5.](#page-4-0) Many researchers work on the effective atomic number and effective electron density of the C H N O based biological material. The data on the effective atomic number for selected amino acid tabulated in the [Table 7](#page-4-1) which shows variations in theoretical and experimental calculated value. Systematic behaviour is shown graphically in [Fig. 7](#page-5-0). This data compare with [Kumar and Reddy \(1997\)](#page-7-32), theoretically we gave the same explanation. We represent the linearly fitting for finding the accurate pick point of the material with energy using the ORIGIN 2016 professional software and it has observed that the value of Z_{eff} is independent shows no effect of photons at selected region. Manohara et al., studied the value of Z_{eff} decreases with increasing energy of three dominant interaction process (photoelectric, Compton and pair production). The result displays no change or variation of Z_{eff} with selected energy region because of the multiple scattering, this shows Compton scattering is dominating and the higher energy value of Z_{eff} is linearly decreases. Similarly, [Table 8](#page-5-1) show no change in effective electron density (N_{eff}) with entire selected energy region. Effective electron density (N_{eff}) measuring the probability distribution of electron, we use the gauss fitting method to find the accuracy of peak point for showing the nature of experimentally measured and XCOM value shown in [Fig. 8](#page-5-2). The value of N_{eff} slightly decreasing then the energy increase had no change. [Kumar and Reddy \(1997\)](#page-7-32) showed that the Z_{eff} does not change in the energy range 400–1400 keV. The present results are in good agreement with literature, i.e. the effective atomic number and effective electron density are related to each other [\(More et al., 2016](#page-7-28)). Also [Fig. 9](#page-5-3) shows the experimental value of the Z_{eff} and N_{eff} as a function of energy explain no effect of energy on the material. We agree the given information comparing with the NIST XCOM available data,

Table 8 Effective electron densities, N_{eff} (10²³ electrons/g) for the investigated amino acids.

Fig. 8. Variation of Neff vs energy for DL-Arginine.

Fig. 9. Variation of Z_{eff} and N_{eff} energy for DL-Arginine.

but having little bit error in the analysis. The systematic errors occurring from narrow beam geometry. The intensity fitted in the Gaussian curve to analysis narrow field ([Torikoshi et al., 2007\)](#page-7-17). The studies of electron density in the entire energy range show the electron to have Gaussian distribution in the energy region ([Petwal et al., 2010](#page-7-33)). This data is useful for measure the radial dose of the material.

6. Effect of incident photon energy and penetration depth on EABF

Using G-P fitting method we observed that the significant variation in value of the EABF in the energy range 0.015–15 MeV up to penetration depth 40 mfp shown in [Fig. 10](#page-6-0) (a–d). The intermediate value of EABF is higher in respect with intermediate energy. The energy behaviour like $E_{pe} < E_{comp} < E_{pp}$ shows the photoelectric effect is dominating at low energy. The intermediate value is higher upto 40 mfp in this medium the Compton scattering is main interaction processes because of multiple scattering slowly remove the photon this occur higher

Fig. 10. Variation of the energy absorption buildup factor with photon energy for selected amino acids (A–E) in the energy region 0.015–15 MeV at (a) 1 mfp, (b) 10 mfp, (c) 20 mfp and (d) 40 mfp.

build up factor at intermediate section similarly up to 0.1 MeV energy is increasing buildup factor is decreasing this shows fast removal the photon. The photoelectric and pair production value of energy absorption buildup factor is lower this shows that in this process fast removal the photon occurred. [Fig. 11](#page-6-1) shows gamma ray EABF value of DL-Arginine was lowest at 1 mfp and highest at 40 mfp. The fig shows that the increasing penetration depth also increases the EABF due to increasing the value of Z_{eq} and scattered photon. This sample reflects that the penetration depth was higher in the three interaction process the Compton scattering reveal that linearly increasing EABF.

7. Conclusion

We have reported that the mass attenuation coefficient, molar extinction coefficient, total cross section, total atomic cross section electronic cross section, Z_{eff}, N_{eff} of the selected six amine group biological materials in the energy region 122–1330 keV. The given data have good agreement with comparing NIST XCOM database and EABF of DL Arginine at 0.015–15 MeV. The study of photon interaction studies with biological material at specific energy. This study shows that the attenuation parameter is depending on the thickness and chemical composition of the biological material in the given energy region. The important part of this study is experimentally measured value of effective atomic number and effective electron density cannot show the variation at energy region 122–1330 keV with using Gaussian fitting for accuracy. The value Z_{eq} increases EABF also increases, hence EABF is depend on the chemical composition of material. The highest value of energy absorption buildup factor observes in the middle portion because of multiple scattering (Compton scattering) and lowest values in another two absorption process (photoelectric and pair production). This study gives better understanding of photon build up control in amino acids as well as proteins. We gave the primary data which are useful in medical physics, medical diagnosis, medical dosimetry and researcher working in this field.

Fig. 11. The energy absorption buildup factor for DL-Arginine up to 40 mfp at 0.05–15 MeV.

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