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Determination of Mass Attenuation Coefficients, Effective atomic number and Electron Density of Lumefantrine in the Energy Range 1 keV – 100 GeV

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Abstract

The effective atomic number and electron density of Lumefantrine(LU) have been calculated for total and partial photon interactions by the direct method in the wide energy range of 1 keV – 100 GeV using WinXCOM. The values of these parameters have been found to change with energy. The variations of effective atomic number and electron density with energy are calculated and shown graphically.

Keywords: LU; Mass attenuation coefficients; Effective atomic number; Electron density.

1. Introduction

Mass Attenuation Coefficients (μ/ρ), Effective atomic number (Z_{eff}) and Electron Density (N_{el}) are important parameters in determining the interactions of X-rays and gamma photons in matter (Manohara & Hanagodimath, 2007). By the large applications and extensive use of gamma-active isotopes in medicine, industry and agriculture, the study of absorption of gamma rays with biological materials is essential in radiation medicine and in the medical field. Mass attenuation coefficient is a measure of how strongly a substance absorbs or scatters radiation at a given wavelength per unit mass per unit area. The knowledge of mass attenuation coefficients of X-rays and gamma photons in biological and other important materials is of significant interest for industrial, biological, agricultural and medical applications (Jackson & Hawkes, 1981). In composite materials, the energy delivered through the photon interactions, a single number cannot represent the atomic number uniquely across the entire energy range, as in case of pure elements. This number for composite materials is known as "effective atomic number" (Z_{eff}) and it varies with energy as pointed out by G. J. Hyne (Hyne, 1952). On the other hand, the concept of z-dependence of photon attenuation coefficient has been utilized in many applications of radiation studies. And it is very important to evaluate the amount of radiation especially in medical Physics (Shivalinge Gowda et al. 2004).

In this study we used the computational technique developed by the Manohara S. R. (Manohara et al. 2008 "a") using the interpolation program WinXCom (Gerward et al. 2001) and its underlying cross-section database for calculating the Z_{eff} of biomolecules. This prompted us to undertake a rigorous and exhaustive investigation of Z_{eff} and N_{el} over an extended energy range 1 keV – 100 GeV. The energy absorption in a given medium can be calculated if certain constants are known, these necessary constants are Z_{eff} and N_{el} of the medium. The importance of this paper from diagnostic or therapeutic point of view is that while calculating the Z_{eff} of the compound, especially when the photon energy is close to the binding energy of the electron present in the compound, it gives correct information about corrections to be added while calculating the dose to the patient. In such cases the experimental determined Z_{eff} may not be agreeable with the theoretical values. In this paper we reported the results on Z_{eff} and N_{el} for LU in the extended energy range from 1 keV – 100 GeV.

2. Computational method and theoretical basis

2.1. Calculation of effective atomic number and electron density.

The total cross- section (σ) per atom in turn can be related as the sum of partial cross sections,

$$\sigma = \sigma_{pe} + \sigma_{pair} + \sigma_{coh} + \sigma_{incoh} + \sigma_{trip} + \sigma_{ph,n,} \quad (1)$$

Where σ_{pe} (or τ), σ_{inch} and σ_{coh} are the photoelectric cross section, incoherent (Compton) and coherent (Rayleigh) cross sections respectively. σ_{trip} (or k_n) and σ_{trip} (or k_e) are the cross sections for electron-positron pair production (creation) in the field of nucleus and in the field of atomic electrons ('triplet production'), respectively. $\sigma_{ph,n}$ is the photo nuclear cross section.

$$\sigma_m = \sum_i n_i \sigma_i \quad (2)$$

where, σ_i and n_i are the number of atoms and atomic cross section of the i^{th} constituent element present in a molecule . σ_i is the mass attenuation coefficient, $(\mu/\rho)_I$ through

$$\sigma_i = \frac{A_i}{N_A}\left(\frac{\mu}{\rho}\right)_i \quad (3)$$

where, N_A is the Avogadro constant and A_i is the atomic mass of the i^{th} element present in a molecule.

The cross section per molecule can be written in terms of an effective (average) cross section per atom, $\sigma_{a,}$ and an effective (average) cross section per electron, $\sigma_{e,}$ as

$$\sigma_m = n\sigma_a = nZ_{eff}\sigma_{e,} \quad (4)$$

Where, Z_{eff} is the effective atomic number and $n = \Sigma_i n_i$ is the total number of atoms present in a molecule.

Equ. (4) can be regarded as the definition of the effective atomic number. Essentially it is assumed that the actual atoms of the molecule can be replaced by the same number of identical (average) atoms, each having Z_{eff} is given by

$$Z_{eff} = \frac{\sum_i n_i A_i \left(\frac{\mu}{\rho}\right)_i}{\sum_i n_i \frac{A_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i} \quad (5)$$

where, Z_i is the atomic number of the i^{th} element present in a molecule.

The effective electron density, $N_{el,}$ can be expressed in the number of electrons per unit mass is closely related to the Z_{eff}, for a chemical element, the electron density is given by $N_{el} = N_A (Z/A)$, this expression can be generalized to a compound, and one has

$$N_{el} = N_A \frac{nZ_{eff}}{\sum_i n_i A_i} = N_A \frac{Z_{eff}}{\langle A \rangle} \quad (6)$$

where, <A> average atomic mass of the compound.

In the present work, we have calculated mass attenuation coefficient and photon-interaction cross sections in the energy range from 1 keV to 100 GeV using WinXCom (Gerward et al. 2004). This program uses the same underlying cross-sectional database as the well known tabulation of Hubbell and Seltzer (1995). WinXCom makes it possible to export the cross-sectional data to a

predefined MS Excel template, a feature that greatly facilitates the subsequent and numerical data analysis.

Table 1.Compound studied in the present work. <Z> is the mean atomic number calculated from the chemical formula. SN is the sample number.

SN	Compound	$\langle Z \rangle$
1	LU	3.52

2. Results and Discussion

2.1. Total photon interaction (with coherent).

The mass attenuation coefficients values for LU are calculated at photon energies 1keV -100 GeV. **Fig-1** shows the variation of mass attenuation coefficients of LU with photon energy in the range 1 keV to 100 GeV. From **Fig-1,**

i) We can see that there are three energy ranges where photo electric absorption, Compton scattering, and pair production respectively, are the dominating attenuation processes. It is seen that the $(\mu/\rho)_c$ values are large and show a decreasing trend with strong energy dependence in the low incident photon energy range of 1 keV- 25 keV. In the intermediate (25 keV) and high (1 MeV) energy regions,

ii) $(\mu/\rho)_c$ values show less energy dependent behavior and gradually decrease with increasing incident photon energy is due to the coherent scattering which varies as Z (Shastry & Jnanananda, 1958) . In the inter mediate energy region, where incoherent scattering is the most dominant process, the mass attenuation coefficient is found to be constant and is due to the linear z-dependence of incoherent scattering and insignificant role played by pair production. In the higher region the variation of mass attenuation coefficient is due to the z dependence of pair production (El-Kateb & Abdul Hamid, 1991).

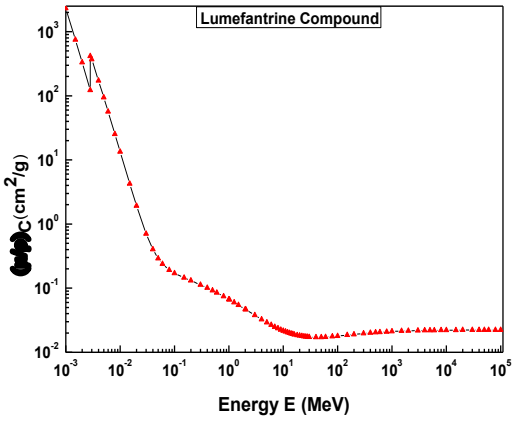

Figure-1. Variation of photon mass attenuation coefficient $(\mu/\rho)_C$ of LU with photon energy for total photon interaction (Coherent).

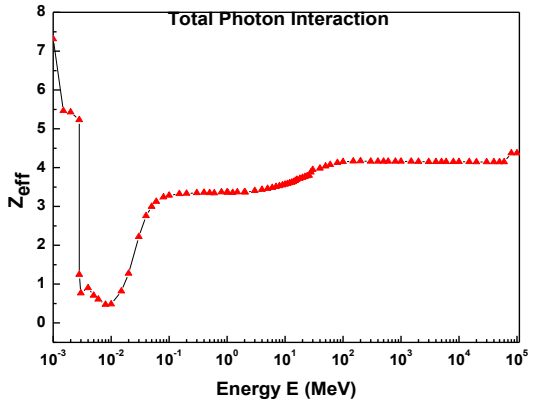

Figure-2. Variation of effective atomic number Z_{eff} of LU with photon energy for total photon interaction (Coherent).

2.2. Photo electric absorption

The variation of Z_{eff} with photon energy for photoelectric absorption is as shown in **Fig.3** which indicates that Z_{eff} is almost of independent of photon energy and remains constant .This is due to the fact that, Photoelectric effect process is predominant at low energies (<1 MeV) and for materials of higher atomic numbers than for low Z materials. Similar results were also obtained by Perumallu et al (Perumallu et al. 1985) in multi element materials of biological importance. The variation of Z_{eff} is almost independent of energy. This is because of the fact that LU consist of elements which are close to atomic number and are same in number.

2.3. Incoherent (Compton) scattering

The variation of Z_{eff} with photon energy for incoherent scattering is as shown in **Fig.4** which indicates that Z_{eff} increases slowly with increase in energy in the region 1-400 keV. Beyond 400 keV, Z_{eff} is independent of photon energy. Most of the elements in a composite material have a value of Z/A of about 0.5 where as hydrogen has a value of 1.0, which effects Compton scattering. This result is similar to the results obtained by S. R. Manohara et al. (Manohara & Hanagodimath, 2007). Khayyoom and Parthasaradhi have also studied Z_{eff} of some alloys; their experimental results suggest that in incoherent scattering Z_{eff} is independent of photon energy from 20 to 800 keV. In our findings Z_{eff} is independent of photon energy only above 400 keV but depends on photon energy below 400 keV. The variation of Z_{eff} depends on respective proportion and range of atomic numbers of the elements of LU.

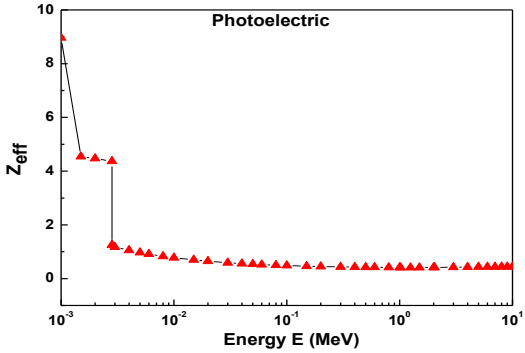

Figure-3. Variation of effective atomic number Z_{eff} of LU with photon energy for photoelectric absorption.

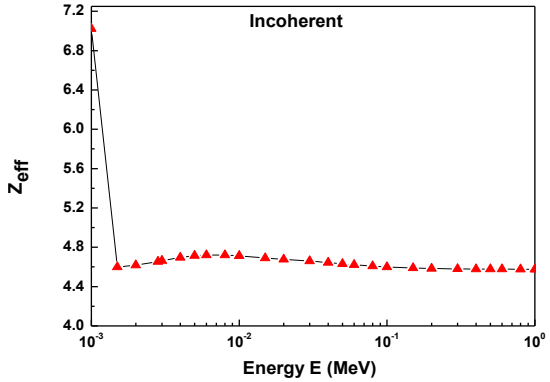

Figure-4. Variation of effective atomic number Z_{eff} of LU with photon energy for incoherent scattering.

2. 4. Coherent (Rayleigh) scattering

The variation of Z_{eff} with photon energy for coherent scattering is as shown in **Fig 5.** From this figure it is clear that Z_{eff} increases with increase in energy from 1 keV to 300 keV, beyond 300 keV Z_{eff} is independent of energy i.e. remains invariable with the increase in energy. Whereas at 200 keV there is a slight steady state and further increase with increase in energy this is due to the presence of sulfur. Our results are in good agreement with the results shown by (Manohara & Hanagodimath, 2007).

2. 5. Pair production (Nuclear field)

The variation of Z_{eff} with photon energy for pair production is as show n in **Fir 6.** With reference to the figure it clears that Z_{eff} is decreases more with increase of photon energy from 1.1 to 100 MeV, this is because of the large number of atomic numbers, beyond 100 MeV there is a slight increase in Z_{eff} is with increase in photon energy and again there is a decrease in Z_{eff} with increase in Photon energy up to 200 MeV and then it remains invariant i.e. independent of photon energy.

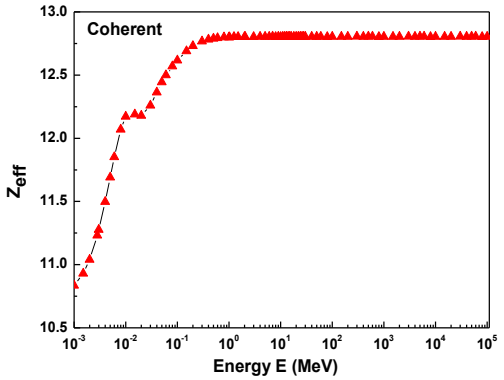

Figure-5. Variation of effective atomic number Z_{eff} of LU with photon energy for coherent scattering.

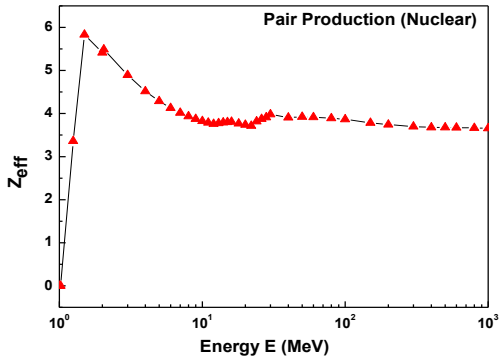

Figure-6. Variation of effective atomic number Z_{eff} of LU with photon energy for pair production in nuclear field.

2.6. Pair production (Electric field)

The variation of Z_{eff} with photon energy for pair production is as shown in **Fig 7.** From the figure it is clear that Z_{eff} slightly decreases 1.1 MeV to 120 MeV and is remains invariant i.e. independent of photon energy from 120 MeV. The variations of N_{el} with photon energy in LU for partial and total interaction processes are similar to that of Z_{eff} and can be explain on the similar manner as that of Z_{eff} and are as shown in **Figs.8-13.**

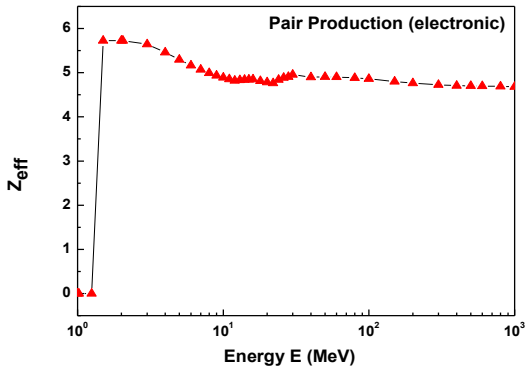

Figure-7. Variation of effective atomic number Z_{eff} of LU with photon energy for pair production in electric field.

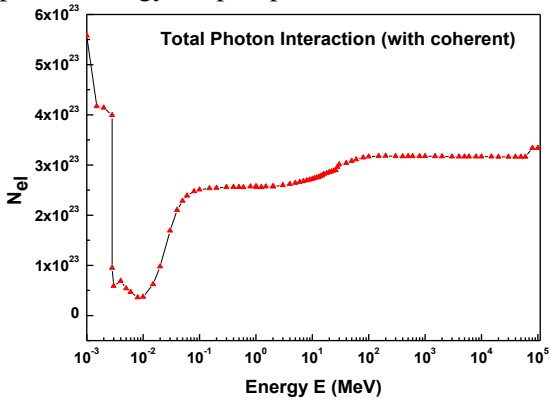

Figure-8. Variation of electron density N_{el} of LU with photon energy for total photon interaction(with coherent).

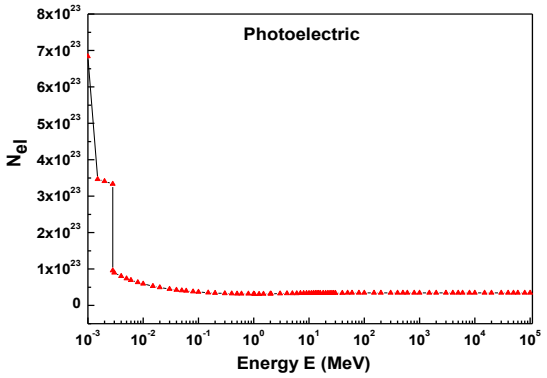

Figure-9. Variation of electron density N_{el} of LU with photon energy for photoelectric absorption.

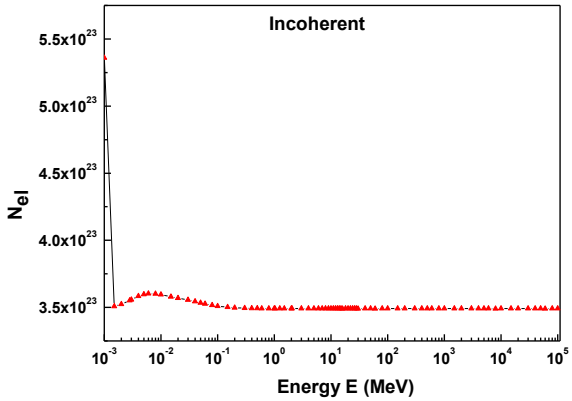

Figure-10. Variation of electron density N_{el} of LU with photon energy for incoherent scattering.

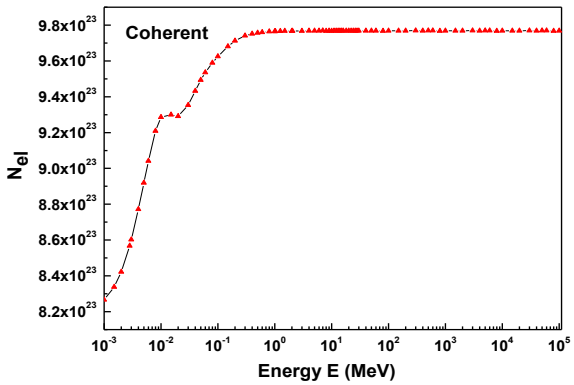

Figure-11. Variation of electron density N_{el} of LU with photon energy for coherent scattering.

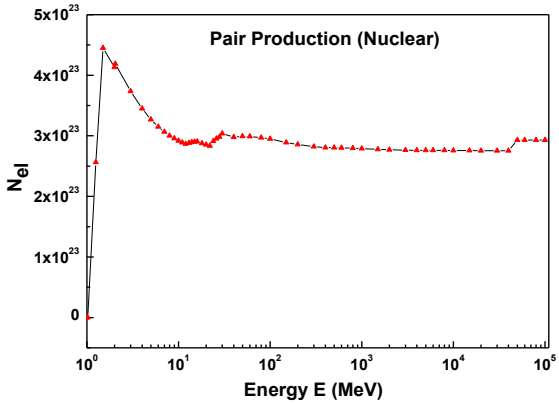

Figure-12. Variation of electron density N_{el} of LU with photon energy for pair production in nuclear field.

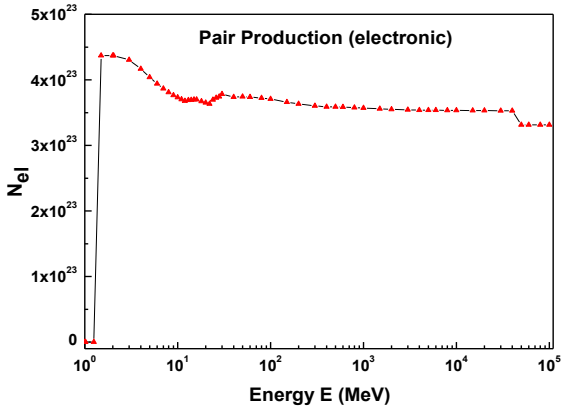

Figure-13. Variation of electron density N_{el} of LU with photon energy for pair production in electric field.

3. Conclusions

1) The Z_{eff} and the corresponding N_{el} of LU have been calculated in the energy region from 1 keV to 100 GeV using WinXcom (Gerward et al. 2001, 2004) and its underlying database of atomic photon interaction cross-sections. We have used a comprehensive and consistent set of formulae i.e. valid for all types of materials and for all energies greater than 1 keV (Manohara et al. 2008 "a").

2) One can distinguish three energy regions of a LU. The three energy regions are approximately E<0.1 MeV, 0.1 MeV<E<100 MeV and E>100 MeV. The main photon interaction processes in these regions are photoelectric absorption, incoherent (Compton) scattering and pair production, respectively. Between these energy regions there are transition regions with a rapid variation of Z_{eff} and N_{el}.

3) The K-absorption edge is found at 2.82 keV with Z_{eff} = 5.23 in the photoelectric absorption region.

4) Z_{eff} and N_{el} are increases for low energies and remains constants for higher energies in coherent scattering. Whereas they decreases for low energies and remains constant for higher energies in case of photoelectric absorption and incoherent scattering respectively.

4. Acknowledgement

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