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Measurements of mass attenuation coefficient, effective atomic number and electron density of some amino acids

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HIGHLIGHTS

- We report the values of mass attenuation coefficients (μ/ρ).
- The values of (Z_{eff}) i.e. effective atomic number are calculated.
- Measurement of effective electron density (N_{eff}) of some amino acids.
- Comparison of all μ/ρ values with XCOM programme.

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ABSTRACT

The mass attenuation coefficients of some amino acids, such as DL-aspartic acid-LR($C_4H_7NO_4$), L-glutamine ($C_4H_{10}N_2O_3$), creatine monohydrate LR($C_4H_9N_3O_2H_2O$), creatinine hydrochloride ($C_4H_7N_3O \cdot HCl$) L-asparagine monohydrate($C_4H_9N_3O_2H_2O$), L-methionine LR($C_5H_{11}NO_2S$), were measured at 122, 356, 511, 662, 1170, 1275 and 1330 keV photon energies using a well-collimated narrow beam good geometry set-up. The gamma-rays were detected using NaI (Tl) scintillation detection system with a resolution of 0.101785 at 662 keV. The attenuation coefficient data were then used to obtain the effective atomic numbers (Z_{eff}), and effective electron densities (N_{eff}) of amino acids. It was observed that the effective atomic number (Z_{eff}) and effective electron densities (N_{eff}) initially decrease and tend to be almost constant as a function of gamma-ray energy. Z_{eff} and N_{eff} experimental values showed good agreement with the theoretical values with less than 1% error for amino acids.

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1. Introduction

Investigation of radiation effects on biologically important molecules find immense applications in the field of medical physics and radiation biophysics. The study of photon interactions with matter is important and the data on the transmission and absorption of X-rays and gamma-rays in biological shielding and dosimetric materials assumed great significance by virtue of their diverse applications in the field of medical physics and medical biology Kaewkhao et al., 2008. A large number of photon attenuation measurements and calculations have been made for different materials and the attenuation coefficient has been studied as a function of different parameters. The attenuation coefficient measurement studies have to give more attention to materials of biologically interest in the energy range 5–1500 keV.Gamma radiations in the energy region above 200 keV up to about 1500 keV interact with matter predominantly by photoelectric effect and Compton effect. The photon interaction cross-section can be expressed as a function of the photon energy and the atomic number Z. At a given photon energy, the interaction cross section is proportional to Z^n where n is expected to be between 4 and 5 for the photoelectric effect, 1 for the Compton effect, and 2 for pair production Henriksen and Baarli, 1957. It is often found convenient to represent the gamma-ray interaction properties of a composite material consisting of a number of different elements in varying proportions by an effective atomic number Z_{eff}. This number depends on the incident energy as well as the atomic number of the constituent elements. It indicates on average, the number of electrons of the material that actively participate in the photon–atom interaction. Hence, the Z_{eff} is used frequently in calculations of mass energy absorption coefficients and Kerma in radiation dosimetry Manjunathaguru and Umesh, 2009. This parameter is also used in the calculation of Compton profiles of complex materials and hence may yield valuable information about the chemical environment that surrounds the atom in a quantitative manner. Hine (1952) pointed out that there is a different atomic number for each interaction process in a complex material.

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In order to make use of the fact that scattering and absorption of gamma-radiations are related to the density and effective atomic numbers of the material, knowledge of the mass attenuation coefficients is of prime importance. From the mass attenuation coefficient, a number of related parameters can be derived, such as the mass energy-absorption coefficient, the total interaction cross-section, the effective atomic number and the effective electron density. The mass attenuation coefficient, μ/ρ, is a measure of the average number of interactions between incident photons and matter that occur in a given mass per unit area thickness of the substance encountered. Early calculations of effective atomic numbers were based on parameterization of the photon interaction cross-section by fitting data over limited ranges of photon energy and atomic number Jackson and Hawkes, 1981. Today, using accurate databases of photon interaction cross-sections and interpolation programs (Gerward et al., 2001, 2004 and Berger and Hubbell, 1987, it is possible to calculate effective atomic numbers with much improved accuracy and information content over wide ranges of photon energy and elemental composition. A simple and widely used method of obtaining Z_{eff} of a composite material consisting of different elements in definite proportions is based on the determination of total attenuation coefficients for gamma-ray interactions by the transmission method. In the present work, the method of deriving effective atomic numbers in composite materials was followed by using the experimental results of mass attenuation coefficients. Experimental results were compared with theoretical values.

A variety of physiological functions inside living systems are performed by complex molecules such as carbohydrates, proteins, fats and oils composed of H, C, N and O elements. Photons of energy from 1500 keV down to about 5 keV are widely used in medical and biological applications, Hubbell, 1999, especially during diagnosis and therapy. A thorough knowledge of the nature of interaction of these biologically important complex molecules such as amino acids is desirable over this energy region. Hence, in recent years, this has motivated many investigators over the years to determine the total attenuation cross-sections as well as composition dependent quantities such as effective atomic numbers (Z_{eff}), and effective electron densities (N_{eff}) of such complex molecules of biological interest in this energy region by employing different methods (Kirby et al., 2003; Midgley, 2004, 2005; Shivaramu, 2001); Shivaramu et al., 2001); Sandhu et al., 2002; Gowda et al., 2004, 2005; Manjunathaguru and Umesh, 2006; Manohara and Hanagodimath, 2007; El-Kateb and Abdul-hamid, 1991).

Theoretical values for the mass attenuation coefficients can be found in the tabulation by Hubbell and Seltzer (1995). A convenient alternative to manual calculations, using tabulated data, is to generate attenuation data, as needed using a computer. For this purpose Berger and Hubbell (1987) developed XCOM software for calculating mass attenuation coefficients or photon interaction cross-sections for any element, compound for a wide range of energies.

There have been a great number of experimental and theoretical investigations to determine mass attenuation coefficients for complex biological molecules such as carbohydrates, proteins, fats and oils composed of H, C, N and O elements in varying proportions. Sandhu et al. (2002) have investigated fatty acids in the energy region 81–1330 keV. Gowda et al. (2004, 2005) have reported total attenuation cross-sections for sugar and amino acids. Recently Manjunathaguru and Umesh (2006), Manohara and Hanagodimath (2007), have determined the effective atomic numbers of several biomolecules. Measurements on the sample containing H, C, and O in the energy range 54–1333 keV have been reported by El-Kateb and Abdul-hamid (1991). In this work, we have measured the mass attenuation coefficients, the atomic cross-sections, the effective atomic numbers, molar extinction coefficients and the effective electron densities for H, C, N and O based amino acids in the energy range 122–1330 keV, and then compared these experimentally evaluated parameters with theory using XCOM program.

2. Theory

In this section we summarize some theoretical relations that have been used for the determination of mass attenuation coefficients in the present work. When a monochromatic beam of gamma photons is incident on a target, some photons are emitted due to the dominant interaction processes and therefore, the transmitted beam is attenuated. The extent of attenuation depends on given elemental target. This attenuation of the beam is described by the following equation:

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

where I_0 and I are the incoming and attenuated photon intensities, respectively μ (cm^{-1}) is the linear attenuation coefficient of the material and t (cm) is the sample thickness. Rearrangement of Eq. (1) yields the following equation for the linear attenuation coefficient:

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

In Eq. (2), the mass attenuation coefficients μ/ρ ($cm^2\ g^{-1}$) for the samples were obtained from Eq. (3) by using the density of the corresponding samples:

$$\mu_m = \frac{\mu}{\rho}(cm^2\ gm^{-1}) = \frac{1}{\rho t}\ln\left(\frac{I_0}{I}\right) \tag{3}$$

where ρ (g/cm^3) is a measured density of the corresponding sample, and I_0 and I are the unattenuated and attenuated photon intensities, respectively.

If the materials are composed of different elements in varying proportions, then it is assumed that the contribution of each element of the compound to the total interaction is additive, yielding the well known mixture rule of Hubbell and Seltzer (1995) that represent the total mass attenuation coefficient $(\mu/\rho)_T$ of any compound as the sum of the appropriately weighted proportions of the individual atoms.

The mass attenuation coefficient, for a compound or mixture is given by:

$$\mu_m = \sum i W_i(\mu_m)_i \tag{4}$$

where W_i and $(\mu_m)_i$ are the weight fraction and mass attenuation coefficient of the ith constituent element, respectively. For a chemical compound the fraction by weight (W_i) is given by:

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

where A_i is the atomic weight of the ith element and n_i is the number of formula units. The values of the mass attenuation coefficients were used to determine the total molecular cross-section ($\sigma_{t,m}$) from the following relation:

$$(\sigma_{t,m}) = \mu_m(M/N_A) \tag{6}$$

where $M = \sum_i n_i A_i$ is the molecular weight of the compound, N_A is the Avogadro's number, n_i is the total number of atoms in the molecule and A_i is the atomic weight of the ith element in a molecule. The total atomic cross-sections ($\sigma_{t,a}$) has been determined from the following equation:

$$(\sigma_{t,a}) = \frac{1}{N_A}\sum_i f_i A_i(\mu_m)_i \tag{7}$$