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Effect of weight fraction of different constituent elements on the total attenuation coefficients of some biologically important compounds

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ABSTRACT

The total attenuation coefficients, μ/ρ, of some biologically important vitamins containing H, C, N and O have been studied as a function of weight fraction of constituent elements. A considerable change in μ/ρ is seen only in low energy region whereas no change is observed with the increasing percentage of constituent elements (hydrogen, carbon, oxygen and nitrogen) in high energy region up to 1500 keV.

Keywords: Weight fraction; attenuation coefficient; biological material.

INTRODUCTION

Data on the transmission and absorption of x-rays and gamma rays in biological, shielding and dosimetric materials assume great significance by virtue of their diverse applications in the field of medical physics and radiation biology.Hydrogen, carbon, nitrogen and oxygen are major constituent elements of the building blocks of carbohydrates, proteins, lipids, enzymes, vitamins and harmones. Photons of energy from 1500keV down to about 5keV are widely used in medical and biological applications [1] Therefore, a thorough knowledge of the nature of interaction of biologically important complex molecules such as carbohydrates, proteins, lipids, enzymes, vitamins and harmones is desirable over the energy region 5-1500 keV. In recent years, several investigators have studied the nature of interaction of such biologically important molecules with photons in this energy regime [2-8].

The penetration and diffusion of radiation in body can be characterized by the study of a parameter namely photon attenuation coefficient. 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 5-1500keV.

This work gives variation of attenuation coefficient data as a function of weight fraction of different constituents of biologically and medically important compounds like vitamins. Similar work on other H, C, O and N based biologically important compounds have been reported by several workers earlier [2-8] .To our knowledge no reports have been found on vitamins with H, C, O and N as their constituent elements. In addition to this objective it is necessary to understand the nature of interaction of γ-rays with these vitamins with the photons of energy 1500keV down to 5keV which are used in medical application.

Among the various biological materials viz amino acids, fatty acids, proteins carbohydrates etc, the vitamins perform important roles in various physiological functions in the human body. Vitamins are compounds which are vital to our health and longevity. Our body needs these vitamins for growth, function, energy, tissues repair and waste removal.

The work reported here is an attempt to incorporate the physics of photon-atom interactions in to a parametrization for the energy and compositional dependence of γ-ray attenuation coefficient and this would assist in identifying the link to the physical parameters that characterize a material (e.g., atomic density and effective atomic number).

This paper presents the results of the theoretical calculations of the total attenuation coefficients, of some vitamins as a function of weight fraction of constituent elements, and variation of effective atomic number with energy E.(hydrogen, carbon, oxygen and nitrogen).

THEORY

Gamma radiation is the electromagnetic radiation emitted in nuclear transitions and its energy lies in the range from a few keV to several MeV. X-rays are emitted in electronic transitions in atoms. Gamma radiations interact with matter predominantly by photoelectric effect, the Compton scattering and pair production process [9] .In the photoelectric effect, the photon is absorbed by a bound electron which is ejected out of the atom .When a photon of energy E_γ interacts with the K shell electron whose binding energy is B_k, the electron is emitted with energy $E_e = E_\gamma - B_k$. Such a process is known as the K shell photoelectric effect. The K shell photoelectric effect is proportional to Z^4/ E_γ^3, where Z is the atomic number of the target; it is significant for high –Z elements and for low energy photons.

In the Compton scattering, a gamma photon interacts with a free electron and transfers part of its energy to the struck electron which is ejected out of the atom. The energy of a scattered photon depends on the angle of scattering. The probability for Compton scattering depends on electron density in the target which is proportional to Z/A, where A is the mass number of the target.

In the pair production process the gamma photon interacts with the Coulomb field of the nucleus and produces an electron–positron pair. The minimum energy required to produce an electron-positron pair is 1.02 MeV, because the sum of rest mass energies of the electron and the positron is 1.02 MeV.If gamma photon energy is greater than 1.02 MeV the excess energy is shared between the electron and the positron in the form of kinetic energy. As the probability of this interaction is proportional to the square of the atomic number of the target, it is predominant in high-Z material.

When a monoenergetic beam of gamma photons is incident on a target, some photons are removed from the beam due to the process mentioned above. Thus the transmitted beam is attenuated. The extent of attenuation depends, for the given elemental target, on the photon energy. If a beam of monoenergetic gamma photons of intensity I_0 is incident on a target of thickness t, the transmitted intensity I_t decreases exponentially as [10]

$$I_t / I_0 = e^{-\mu t} = e^{-\mu/\rho(t)} = e^{-N\sigma} , \qquad (1)$$

where μ (cm^{-1}) is the linear attenuation coefficient , μ/ρ(cm^2 g^{-1}) is the mass attenuation coefficient, t (cm) is the thickness of the target, ρt (g cm^{-2}) is the mass thickness , σ(cm^2) is the atomic cross section and N is the number of atoms per cm^2 of the target. The linear attenuation coefficient μ is the probability per unit length that an incident gamma photon interacts with the target material, the mass attenuation coefficient μ/ρ is the probability per unit areal density that an incident gamma photon interacts with the target material, and σ is the cross section offered by an atom for interaction with the incident gamma photon. By determining experimentally I_t and I_0 for a given target thickness t, one can determine μ/ρ using relation:

$$\mu / \rho = t^{-1} \ln (I_0/ I_t). \qquad (2)$$

The total atomic cross section σ_{tot} is related to μ/ρ by

$$\sigma_{tot} (cm^2/g) = \mu/\rho \, (cm^2/g) \times u \, (g) \times A , \qquad (3)$$

where u (g) is the atomic mass unit which is (1/12) th of the mass of the carbon atom (1.6605402 x 10^{-24} g) and A is the atomic weight of the target element. The total atomic cross section σ_{tot} is the sum over the cross sections for the photoelectric effect, the Compton scattering and pair production processes.

In this work an attempt has been made to study the effect of H, C, N, and O weight fractions on the mass attenuation coefficients,μ/ρ, of biological materials such as vitamins which are listed in table 1.

The mass attenuation coefficients, μ/ρ, of biological materials such as vitamins have been computed in the energy range 10 keV to 1500keV using a software program [11].

Table 1. Effective atomic number Z_{eff} and change in weight fraction of H, C, O and N of vitamins.

Material	Effective atomic number Z_{eff} at					Change in weight fraction of			
	6.4keV	13.95 keV	17.74 keV	24.14 keV	81 keV	H%	C%	O%	N%
Vitamin B_3 $C_6H_5NO_2$	1.73	1.63	1.30	0.86	0.02	35.71	42.86	14.23	7.14
Vitamin B_9 $C_{19}H_{19}N_7O_6$	1.27	1.18	0.89	0.54	0.01	37.25	37.25	11.76	13.73
Vitamin C $C_{20}H_{30}O$	1.97	1.88	1.52	1.01	0.04	40.00	30.00	30.00	----
Vitamin B_2 $C_{17}H_{20}N_4O_6$	1.29	1.22	0.92	0.55	0.01	42.55	36.17	12.77	8.51
VitaminB$_1$ $C_{12}H_{17}N_{5O}4S$	1.64	1.57	1.22	0.74	0.01	43.59	30.77	10.27	12.82
Vitamin P $C_{28}H_{34}O_{15}$	1.17	1.09	0.81	0.48	0.01	44.16	36.36	19.48	----
Vitamin K $C_{13}H_{16}CINO$	2.69	2.77	2.36	1.70	0.10	48.48	39.39	3.03	3.03
Vitamin B_6 $C_8H_{11}NO_3$	1.56	1.42	1.08	0.73	0.01	50.00	33.33	8.33	8.33
Vitamin B_5 $C_{18}H_{32}CaN_2O_{10}$	1.84	1.79	1.42	0.91	0.01	53.13	28.13	15.63	3.13
Vitamin A $C_{20}H_{30}O$	1.16	1.09	0.83	0.51	0.01	58.82	39.22	1.96	----
Vitamin D $C_{28}H_{44}O$	1.06	0.99	0.74	0.44	0.01	61.11	37.50	1.39	----
Vitamin E $C_{29}H_{50}O_2$	1.04	0.97	0.73	0.43	0.01	61.73	35.80	2.47	----

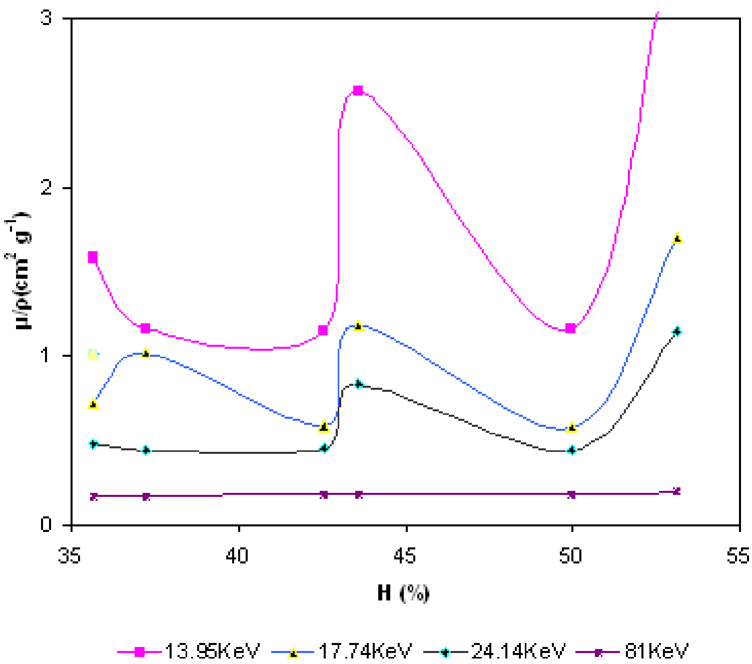

Fig.1 Plot of μ/ρ (cm^2/g) vs. hydrogen weight fraction at some energies for vitamins B_3, B9, B2, B1, B6 andB_5 having increasing H% weight fraction.

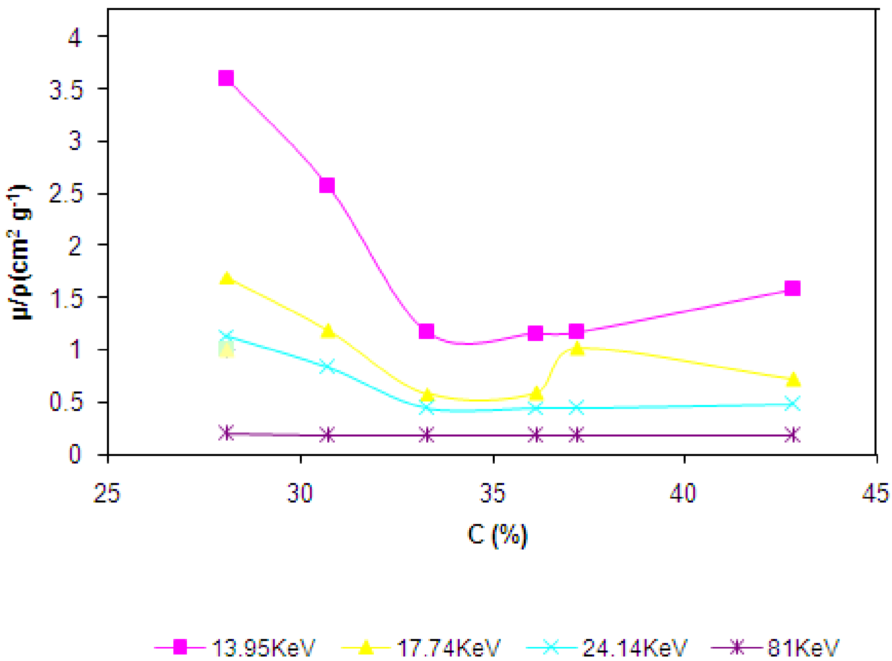

Fig.2 Plot of μ/ρ (cm^2/g) vs. carbon weight fraction at some energies for vitamins B_5, B1, B6, B2, B9 andB_3 having increasing C % weight fraction.

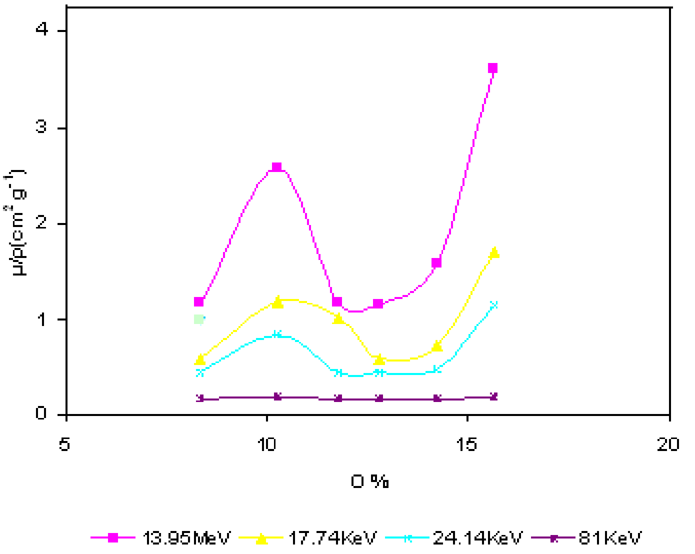

Fig.3 Plot of μ/ρ (cm^2/g) vs. oxygen weight fraction at some energies for vitamins B_6,B_1,B_9,B_2,B_3 andB_5 having increasing O % weight fraction.

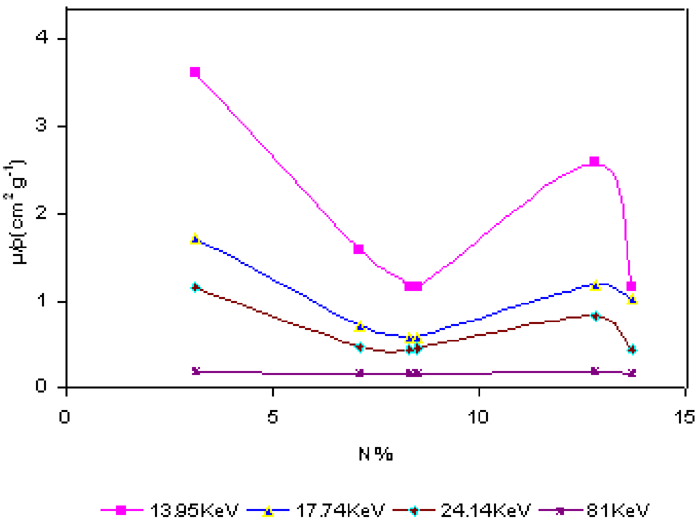

Fig.4 Plot of μ/ρ (cm^2/g) vs. nitrogen weight fraction at some energies for vitamins B_5, B3, B6, B2, B1 and B_9 having increasing N % weight fraction.

RESULTS AND DISCUSSION

The mass attenuation coefficients, μ/ρ, of biological materials such as vitamins were computed in the energy range 5 to 1500 keV. The total interaction cross section of the chosen biological materials were computed with the help of a convenient and state -of -the–art computer program [11] named XCOM: 'Photon cross sections on a Personal Computer', in the energy range 5to 1500keV.The variation of the computed values of μ/ρ due to weight fractions of different constituent elements is shown graphically (Fig.1-4) for the energy range 13.95keV-81 keV as there is no considerable change in σ_{tot} values above 81 keV. Table 1 gives effective atomic numbers (Z_{eff}) and change in weight fraction of H, C, O and N of vitamins. The values of Z_{eff} have been calculated in the present energy range [8].It is observed that the value of Z_{eff} decreases with increase in energy.

Fig.1depicts the plot of μ/ρ (cm^2/g) vs. hydrogen weight fraction for different energies. From this graph, it is seen that at low energy there is a large value of μ/ρ and as energy increases there is a decrease in the value of σ_{tot}. For photon with energy 6.4 keV the μ/ρ is 13.47 cm^2/g where as for 1330 keV photons the μ/ρ value is 0.06 cm^2/g. The variation of μ/ρ with weight fraction is observed for all energies; the μ/ρ values decrease for 35 to 40% hydrogen weight fraction and then increase for 40 to 44% hydrogen weight fraction and after this it goes on decreasing up to 50% hydrogen weight fraction and after this it increases. This is for low energy region (6.4-24.14keV) and for high energy region (81-1330 keV) μ/ρ values are remains nearly constant.

The plot of μ/ρ (cm^2/g) vs. carbon weight fraction at some energies is shown in Fig. 2 In this case at low energies i.e. up to 24.14keV there is a large value of μ/ρ and as energy increases there is a decrease in the value of μ/ρ. For photon with energy 6.4 keV the μ/ρ is 33.9 where as for 1330 keV photons the μ/ρ value is 0.052. The variation of μ/ρ with carbon weight fraction is observed for all energies (6.4-1330keV); for low energy region (6.4 -24.14keV) the μ/ρ value decreases from 28 to 34% and then increases up to 43% carbon weight fraction. For energies from 81keV to 1330keV the μ/ρ values are nearly remain constant from 28 to 43 % carbon weight fraction.

Fig.3 represents a plot of μ/ρ (cm^2/g) vs. oxygen weight fraction at some energies. Here, in the low energy region, there is a large value of μ/ρ and as energy increases there is a decrease in the value of μ/ρ. For photon with energy 6.4 keV the μ/ρ is 13.33cm^2/g where as for 1330 keV photons the μ/ρ value is 0.058 cm^2/g. The variation of μ/ρ with weight fraction is observed for all energies (6.4-1330 keV);); for low energy region(6.4 -24.14keV) the μ/ρ values increase from 8 to 10 % oxygen weight fraction then decreases up to 12% oxygen weight fraction then after this it goes on increasing up to 16 % oxygen weight fraction .For higher energies 81-1330keV the μ/ρ values are nearly remain constant from 8 to 16 % oxygen weight fraction.

Fig. 4 is a plot of μ/ρ (cm^2/g) vs. nitrogen weight fraction at some energies. At low energies up to 24.14keV there is a large value of μ/ρ and as energy increases there is a decrease in the value of μ/ρ . For photon with energy 6.4 keV the μ/ρ is 33.9 cm^2/g where as for 1330 keV photons the μ/ρ value is 0.05 cm^2/g. The variation of μ/ρ with nitrogen weight fraction is observed for all energies (6.4-1330keV); for low energy region (6.4 -24.14keV) the μ/ρ values decrease from 3 to 9% nitrogen weight fraction then after this it goes on increasing up to 13 % nitrogen weight fraction and then decreases up to14 %. For higher energies 81-1330keV the μ/ρ values nearly remains constant for 3 to 14% nitrogen weight fraction.

In the low energy region, compounds containing H, C, N and O behave as incoherent scatterers and that as a consequence of this fact, it is possible to represent the interaction of photons in the low energy region by a single average atomic number (Z_{eff}).In the region below 145 keV down to 5keV, all the three partial interaction processes, namely, photoeffect, coherent scattering and incoherent scattering contribute not too insignificantly to the total interaction. Since these processes exhibit energy dependence characteristically different from one another, their contribution to the total interaction also varies with energy. As a result, the Z_{eff} values are also expected to show energy dependence unlike in the case of energies above 145keV as observed in the present work. The negligible variation in μ/ρ in the high energy region may be due to very small variation in Z_{eff} values above 81keV.

CONCLUSION

The results of this work predict that in low energy region, the total attenuation coefficient, μ/ρ is having higher value and as energy increases μ/ρ value goes on decreasing. It is also observed that for low energy region there is a variation in the total attenuation coefficients values but for high energy region the values of total attenuation coefficients remain constant.

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