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STUDY OF Z_{eff} FOR DNA, RNA AND RETINA BY NUMERICAL METHODS

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The effective atomic number of a biomolecule for photon interaction present in DNA, RNA and retina has been estimated in the energy range 0.001–20 MeV using two different numerical methods. The significant variation of Z_{eff} with photon energy is reported. This shows that Z_{eff} is not constant with energy for photon interaction in DNA, RNA and retinal.

INTRODUCTION

Hine[1] pointed out that the effective atomic number of material composed of various elements for gamma ray interactions cannot be expressed by single number. Bandal and Singh[2] and Kiran Kumar and Venkata Reddy[3] showed that an effective atomic number of biological samples for photon interaction varies with the photon energy. Studies of effective atomic number for photon energy absorption and photon attenuation of tissues from the human organs are carried out by Shivaramu[4].

The first impact of radiation is on individual cells. Radiation can damage the cells by causing ionisations of atoms within the cell, free radical formation within the cell, hydrogen peroxide poisoning of cell and breakage of DNA strands. Ionising radiation will cause ionisations within the cell due to the primary and secondary effects of the radiation. Ionisation of water can lead to the formation of H^+ and OH^- free radicals within the cell that will attack proteins within the cell and that can recombine to form hydrogen peroxide (H_2O_2) that poisons the cell. Finally, the free radicals or the direct radiation can interact with the DNA strands in the nucleus of the cell to cause damage to the information stored there. Under normal circumstances, this damage can be repaired properly but, on occasion, it is either improperly repaired or not repaired at all, leading to errors when the cell reproduces itself. If this damage occurs slowly then it can be repaired as it happens. In the case of a large acute dose, the damage may be extensive enough and in a short enough time frame to be irreversible, resulting in the death of the cell.

Mass attenuation coefficient (μ/ρ) is a measure of probability of interaction (attenuation) that occur between a photon and a matter of unit mass per unit area. The extent to which the biological system is affected due to ionising radiation depends on μ/ρ. DNA and RNA are genetic materials found in chromosomes. Retina is a photoreceptor cell present in rods of the retina. The gamma radiation causes damages to these genetic materials due to radiation-induced mutation in ova and sperm cells and to the retina, which in turn leads to blindness. The estimation of Z_{eff} for these molecule helps in characterising the biomolecule.

DNA and RNA contain pentosesugar, phosphate group and nitrogenous bases (adenine, guanine, cytocine, thymine/uracil). In DNA, adenine (A) is bonding with thymine (T) through double bond (A=T) and guanine (G) bonding with cytocine (C) through triple bond (G=C). The series of (A=T) and (G=C) forms an oligonucleotides leads to DNA. Similarly, series of oligonucleotides formed by the adenine, uracil (U), guanine and cytocine constitute RNA. The long sequence of A, T/U, G and C nucleotides is the repository of genetic information. The stability of DNA and RNA depends on the nitrogenous bases and also the genetic information is carried by them only. Interaction between the photon and the nitrogenous bases is important[5].

When a photon is absorbed by the retina, which is the component of rhodopsin causes the photochemical change, i.e. 11-*cis*-retina is converted into all-*trans*-retina. This change in the structure of the chromophore causes conformational changes in rhodopsin molecule, which is the first stage in the visual transduction. The study of interaction between photon and retina finds importance in medical therapy[3].

Hence in the present study, we are computing the Z_{eff} of photon interaction for basic components of DNA such as adenine, guanine, cytocine, thymine, and basic components of RNA such as adenine, guanine, cytocine, uracil and retina at various photon energies (E) using the following two theoretical methods. Method 1 is used by many of the workers in the past, whereas Method 2 is a recent one.

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METHOD 1

The cross section σ of an element is given by Hubbell and Seltzer[6]

$$\sigma = \frac{\mu/\rho}{A/N}, \quad (1)$$

where, A is the atomic weight of the element and N is the Avogadro number.

Using theoretical values of μ/ρ tabulated by Hubbell and Seltzer[6] for different elements of atomic number (Z) at various E, σ may be estimated for each element at each E. A graph between σ and Z may be obtained.

The mass attenuation coefficient of a compound or a mixture (biomolecule) consists of various elements is given by mixture rule[7]

$$\left(\frac{\mu}{\rho}\right)_{\text{bio}} = \sum_i W_i \left(\frac{\mu}{\rho}\right)_i, \quad (2)$$

where, $(\mu/\rho)_i$ and W_i are mass attenuation coefficient and fractional abundance by weight of ith element present in a molecule, respectively.

The cross section σ_{bio} for $(\mu/\rho)_{\text{bio}}$ of a bio molecule is given by

$$\sigma_{\text{bio}} = \frac{(1/n)(\mu/\rho)}{\sum_i (W_i/A_i)}, \quad (3)$$

where, A_i is the atomic weight of the ith element in a molecule.

Shivaramu[4] estimated $(\mu/\rho)_{\text{bio}}$ for various human tissues and organs using theoretical values of μ/ρ of elements tabulated by Hubbell and Seltzer[6] in expression (2). They estimated σ_{bio} using expression (3) and then Z_{eff} for the above biomolecule at each E by comparing σ_{bio} with the graph of σ versus Z.

METHOD 2

Icelli and Erzeneoglu[8] estimated Z_{eff} of vanadium and nickel compounds for photon interaction as follows.

$(\mu/\rho)_{\text{bio}}$ is given by expression (2) and its molecular cross section σ_{m} is given by

$$\sigma_{\text{m}} = \frac{1}{N}\left(\frac{\mu}{\rho}\right)_{\text{bio}} \sum_i n_i A_i, \quad (4)$$

where, n_i is the number of atoms of ith element in a given molecule.

The atomic cross section σ_{a} is given by

$$\sigma_{\text{a}} = \frac{\sigma_{\text{m}}}{\sum_i n_i}. \quad (5)$$

The electronic cross section σ_{e} is given by

$$\sigma_{\text{e}} = \frac{1}{N}\sum_i \left(\frac{f_i A_i}{Z_i}\right)\left(\frac{\mu}{\rho}\right)_i, \quad (6)$$

where, f_i is the fractional abundance and Z_i is the atomic number of ith element in a molecule, respectively.

The effective atomic number is then given by

$$Z_{\text{eff}} = \frac{\sigma_{\text{a}}}{\sigma_{\text{e}}}. \quad (7)$$

PRESENT WORK

The molecular formulae and compositions of various biomolecules used in the present study are shown in Table 1.

The theoretical Z_{eff} values estimated using both the methods for the various biomolecules at various photon energies ranging from 0.001 to 20 MeV are compared in Figures 1–7.

RESULTS AND DISCUSSION

Figures 1–7 show variation of Z_{eff} with photon energy (E) of biomolecules adenine, guanine, thymine, deoxyribose, retina, cytosine and uracil using both methods. This shows that Z_{eff} is not constant with energy for photon interaction in components of DNA, RNA and retina. The stability of DNA and RNA depends on the nitrogenous bases. Interaction between the photon and the nitrogenous bases leads to the breakage of bonds between adenine with thymine/uracil and guanine with cytocine. In addition, there may be a breakage of bonds with in the nitrogenous bases, which in turn change the alignment of oligonucleotides. Hence, photon interaction changes the Z_{eff}, which may leads to change the biological functions of DNA and RNA. Change in Z_{eff} of retina may also lead to change the biological functions (Lehninger).

Table 1. The molecular formulae of various biomolecules used in the present study.

Biomolecule	Adenine	Guanine	Cytosine	Thymine	Uracil	Deoxyribose	Retina
Molecular formulae	$C_5H_5N_5$	$C_5H_5ON_5$	$C_4H_5ON_3$	$C_5H_6O_2N_2$	$C_4H_4O_2N_2$	$C_5H_{10}O_4$	$C_{20}H_{28}O$

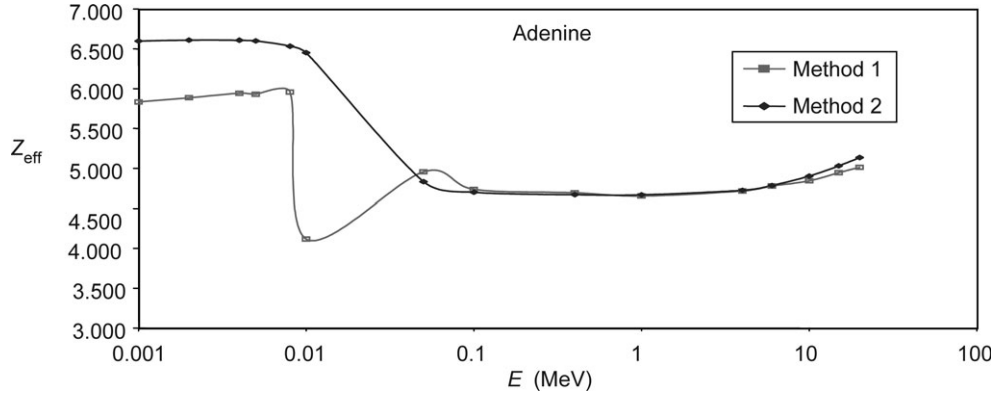

Figure 1. Variation of effective atomic number with energy for adenine.

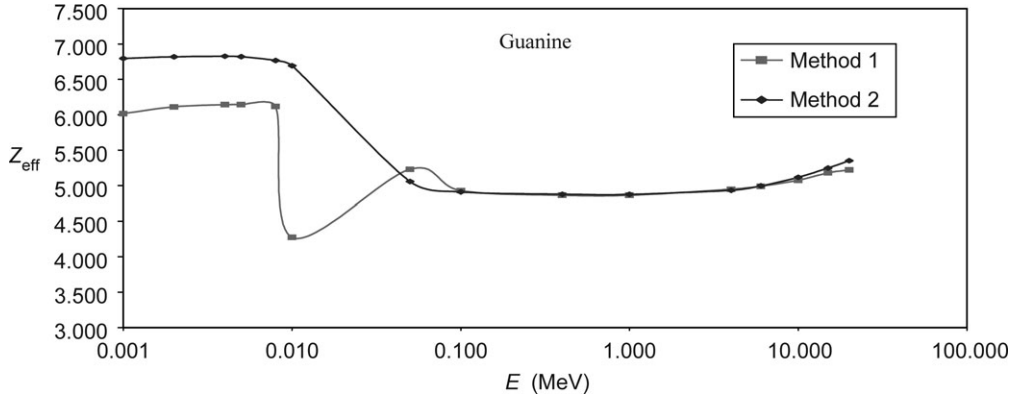

Figure 2. Variation of effective atomic number with energy for guanine.

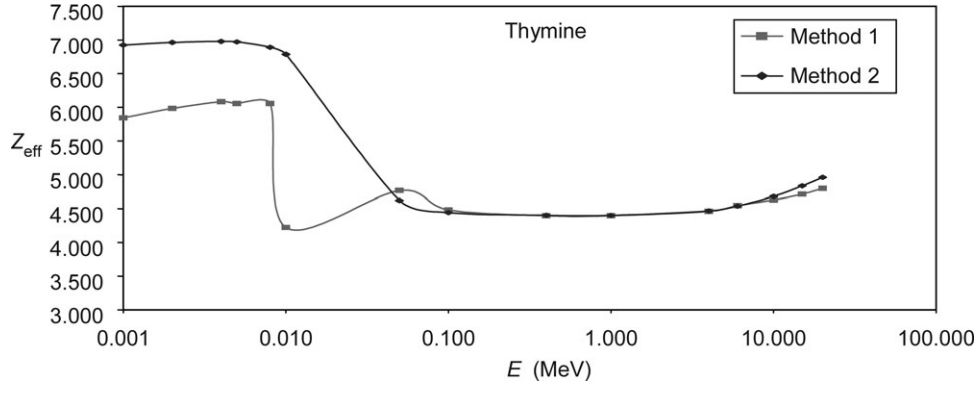

Figure 3. Variation of effective atomic number with energy for thymine.

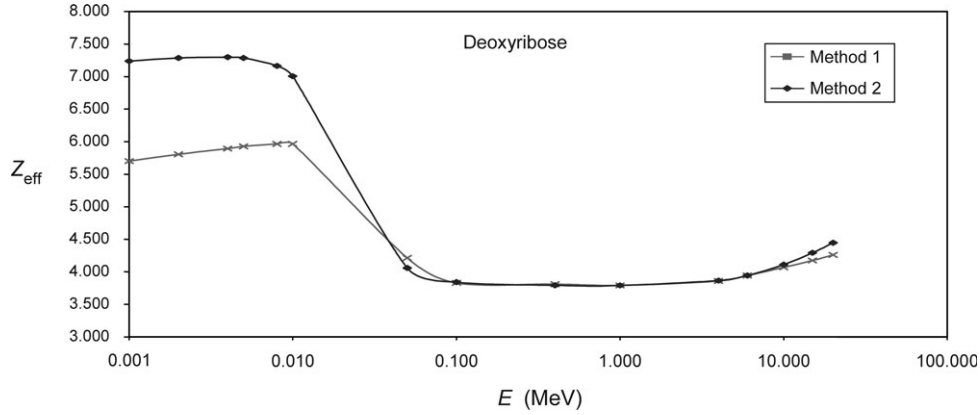

Figure 4. Variation of effective atomic number with energy for deoxyribose.

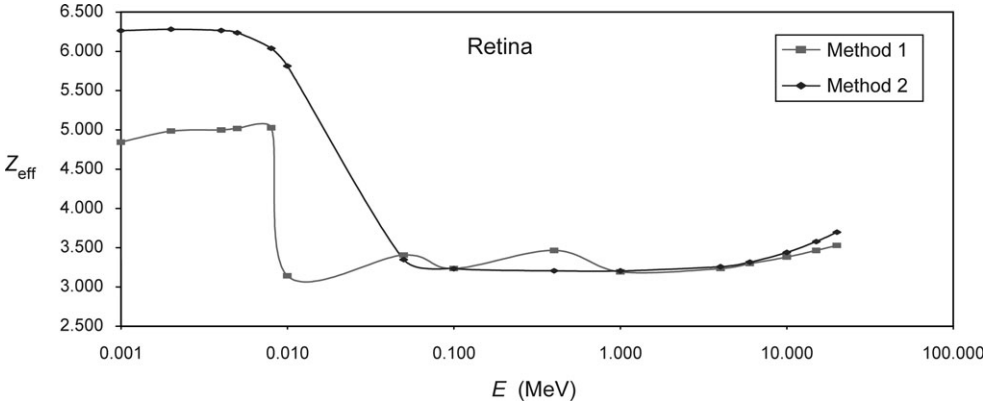

Figure 5. Variation of effective atomic number with energy for retina.

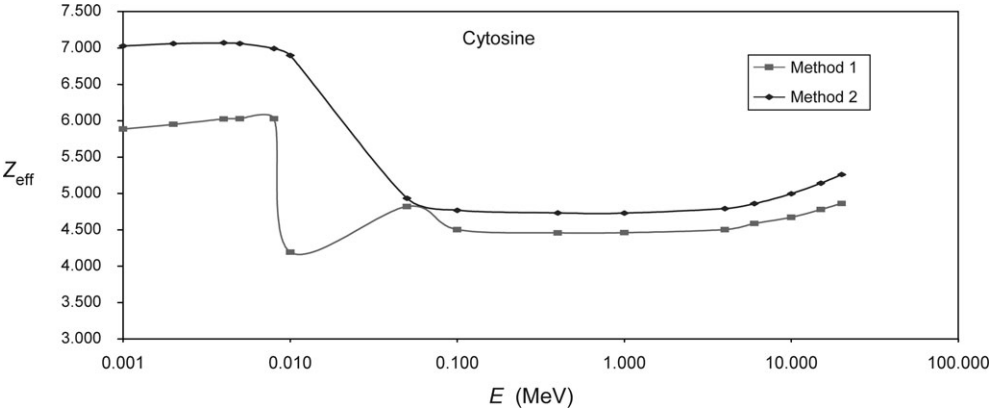

Figure 6. Variation of effective atomic number with energy for cytosine.

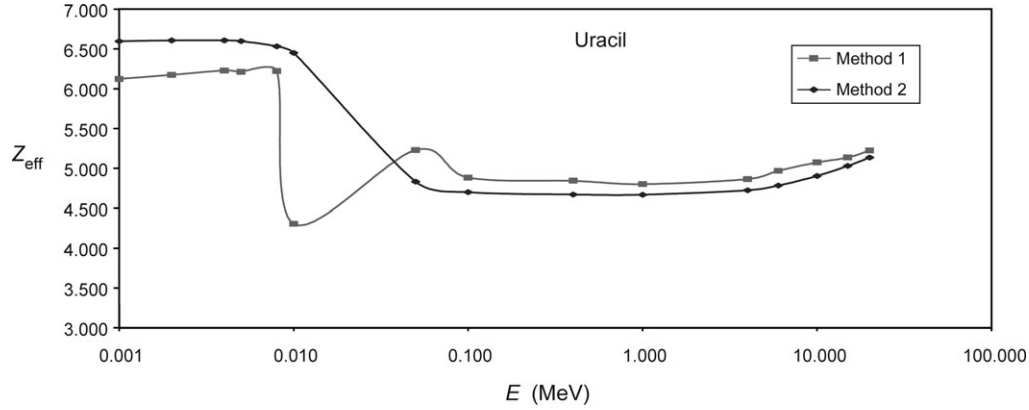

Figure 7. Variation of effective atomic number with energy for uracil.

In the case of nitrogenous bases of DNA and retina (Figures 1–5), it is observed that both methods disagree in the photon energy range 0.001–0.1 MeV for Z_{eff} and agree very well thereafter, except in cytocine (Figure 6) where in, there is a complete disagreement at all energies. For photon energy range 0.001–0.1 MeV, Z_{eff} is found to be higher for Method 2 than Method 1. In case of RNA (Figure 7), same trend is observed as seen in DNA for the photon energy range 0.001–0.1 MeV, thereafter difference is not significant at all energies. Even here, Z_{eff} is found to be higher for Method 2 than Method 1. In both methods, Z_{eff} is found to vary at all energies throughout, as seen by earlier workers.

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