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Effective atomic numbers and electron densities of vitamins containing H, C, N and O.

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ABSTRACT

The total attenuation cross section of biologically important compounds (Vitamins) containing H, C, N and O in the energy range 5-1500 keV have been obtained. Effective atomic numbers (Z_{eff}) and electron densities (N_e) for vitamins have been calculated for different energies. The effective atomic cross sections are the total attenuation cross sections divided by the total number of atoms of all types present in a particular sample. Further, the effective atomic weight is defined as the ratio of the molecular weight of a sample to the total number of atoms of all types in it. The variation of the effective atomic number has been systematically studied with respect to the effective atomic weight. The significant variation of Z_{eff} and N_e is due to the variations in the dominance of different interaction processes in this energy region. The variation of the Z_{eff} values with A_{eff} is studied at all energies of interest. The Z_{eff} values obtained in the energy region of present interest are related to their respective effective atomic weight. It is found that the ratio Z_{eff} / A_{eff} was 0.533 for vitamins containing H, C, N and O elements in the energy region studied.

Keywords: Attenuation coefficient, Electron density, Effective atomic number, Biomolecules, Vitamins, Atomic cross sections.

INTRODUCTION

Investigation of radiation effects on biologically important molecules find immense applications in the field of medical physics and radiation biology. The biologically important molecules perform a variety of physiological functions inside living systems and assist to produce and store energy. These molecules are composed mainly of H, C, N and O elements. Depending upon the quantity of the radiation absorbed by the biological matter, the extent of radiation damage is observed .In biological materials (proteins, nucleic acids, cells and multi-cell organisms) very low doses are sufficient to modify and inactivate the bio molecules.

The various applications of γ-radiation therefore require quantitative and accurate knowledge of the processes by which the photons interact with the atoms of the material and get absorbed. Gamma radiations interact with matter predominantly by photoelectric effect, coherent (Raleigh) and incoherent (Compton) scattering, and, in the photon energy region above 1MeV, pair production process. Photons of energy from 1500 keV down to about 5keV are generally used in medical and biological application. The photons of energies 145.4 keV, 279.2keV,514keV,661.6keV,1115.5keV,1173.2 keV and 1332.1 keV emitted from radioactive sources ^{141}Ce,^{203}Hg,^{85}Sr,^{137}Cs,^{65}Zn and ^{60}C0 are widely used in radiation biology in various applications particularly during diagnostics and therapy[1]. This has prompted us to determine the total attenuation cross sections as well as the composition dependent quantities such as effective atomic numbers Z_{eff} and effective electron densities N_e of molecules of biological interest in the energy region of medical interest at selected energies. It is, therefore, desirable to have a complete knowledge of the nature of interaction of biological molecules over this energy region.

Hence, in recent years, several experimental and theoretical investigations have been carried out to understand the nature of interaction of different biological molecules [2-9].

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. There are two categories of vitamins water-soluble and fat –soluble. All these vitamins are composed of H, C, N and O as their constituent elements. To our knowledge there are no experimental or theoretical results /reports on the gamma ray interaction studies of these vitamins.

The intensity of the incident γ-radiation is attenuated due to its interactions with atomic species which occur during the passage through the material. This attenuation is governed according to the exponential absorption law

$$I(t) = I_0 \exp[-(\mu/\rho)\, t] \qquad (1)$$

where μ/ρ is the mass attenuation coefficient, I_0 and I(t) are the intensities of incident (unattenuated) and transmitted (attenuated) γ-ray photons and t is the mass per unit area of the material. This equation can be used to obtain μ/ρ from measured I_0, I and t data. The mass attenuation coefficients are a measure of the average number of interactions that occur between the incident photons and mass per unit area. These interactions are related to the atomic number of an element and the photon energy for a single element. The three major gamma ray interaction processes viz Photoelectric, Compton and coherent scattering and Pair production can be expressed as a function of photon energy $h\nu$ and atomic number Z of the element. At a given photon energy [7, 10-12] the interaction is proportional to Z^n where n is between 4 and 5 for Photoelectric effect, 1 for Compton effect and 2 for Pair production. In the case of heterogeneous material, consisting of number of elements in varying proportions, it is possible to describe it with the help of a parameter called effective atomic number Z_{eff}.

The idea of effective atomic number is to assume that a compound can for special purposes be regarded as being built up of one kind of species with atomic number Z_{eff} .In materials like biological molecules and other compounds, for photon interaction a single atomic number can not represent the atomic number uniquely across the entire energy region because of the effective atomic number being related to the density and atomic number of an element. It is, therefore, necessary to characterize the interaction processes a single effective atomic number. (Z_{eff}) in the energy region of interest for biologically important compound. The values of Z_{eff} for human tissues and other biological materials have been measured or calculated by several investigators [1, 13-15].

The value of Z_{eff} finds its use in the computation of other useful quantities like the absorbed dose and built up factor. The number Z_{eff} varies with energy; on the other hand, the dependence of Z_{eff} on photon attenuation coefficient has been utilized in many applications of radiation studies. The precise knowledge of effective atomic number is used in radiation dosimetry and medical imaging, when the cross sectional anatomy is generated by computer tomography (CT) scan. Thus a precise knowledge of effective atomic number and electron density of the biologically important compounds is necessary in the energy range of medical interest. To our knowledge there are no reports on the gamma ray interaction studies of vitamins. The aim of the present work is to determine σ_{tot} interaction cross section, effective atomic number and electron density for vitamins which have H, C, N and O as their constituent elements in their different weight proportions in the energy range 5keV-1500keV .The photons in this energy region have immense application in radiation biology a especially during diagnostic and therapy. In the present work, we report the effective atomic number Z_{eff} and electron density N_e values of some H, C, N and O based samples such as vitamins at seven photon energies of 145.4keV, 279.2 keV, 514 keV, 661.6 keV, 1115.5 keV, 1173.2 keVand 1332.1 keV. The effective atomic number, Z_{eff} and the effective electron density N_e have been calculated for vitamins for photon interaction in the energy range from 5-1500 keV using an accurate database of photon–interaction cross section and the WinXCOM program [1].A quantity A_{eff} called the effective atomic weight was calculated as the ratio of the molecular weight of the sample to the total number of all types of atoms present in it. The variation of the Z_{eff} values with A_{eff} was studied at all energies of interest.

2 Theory

A narrow beam of monoenergetic photons is attenuated to intensity I from incident intensity I_0, according to the exponential absorption law (eq.1).The exponential attenuation law (eq.1) can be rewritten as

$$\mu/\rho = t^{-1}\ln [I_0/ I (t)] \quad (2)$$

where μ is the linear attenuation coefficient in $cm^{-1}$and ρ is the density of the absorber in $gm.cm^{-3}$. For a heterogeneous compound composed of various elements, the total attenuation coefficient $(\mu/\rho)_T$ is related to μ/ρ values of constituents by mixture rule [1].

The atomic cross sections are proportional to the probability of photon interactions, and are additive. The total photon interaction cross section σ_{tot} can be written as

$$\sigma_{tot} = \sum_i n_i \frac{A_i}{N_A} (\mu/\rho)_i \quad (3)$$

where N_A is the Avogadro's number,A_i is the atomic mass of the i^{th} element and $(\mu/\rho)_i$ is the mass attenuation coefficient of i^{th} element present in the molecule.

The total cross section σ_{tot} can be expressed in terms of effective cross section per atom, σ_a and an effective cross section per electron σ_e as

$$\sigma_{tot} = n\,\sigma_a = n\,Z_{eff}\,\sigma_e \quad (4)$$

where Z_{eff} is the effective atomic number and $n = \sum_i n_i$ is the total number of atoms present in a molecule. Here it is assumed that the atoms of the molecule can be regarded to have identical atomic number called effective atomic number. The effective atomic number (Z_{eff}) of the compound is related to (μ/ρ) by the following relation [12].

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

where Z_i is the atomic number of the i^{th} element present in a molecule. Other expressions for the effective atomic numbers are found in [16-18] Using the values of Z_{eff}, the effective electron density N_e is calculated using the expression

$$N_e = N_A\,Z_{eff} / A_{eff} \quad (6)$$

where N_A is the Avogadro's number , $A_{eff} = A/n_i$ is the effective atomic weight ,is the ratio of the molecular weight of the sample divided by the total number of the atoms of all types present in the compound.

In the present work, we have generated mass attenuation coefficients and photon-interaction cross sections in the energy range from 5keV -1500keV using WinXCOM. This program uses the same underlying cross-sectional database as the well-known tabulation of [19]. WinXCOM makes it possible to export the cross-sectional data to a predefined MS Excel template, a feature that greatly facilitates the subsequent graphical and numerical data analysis.

The values of effective atomic number Z_{eff} have been calculated using the expression given by [5].

$$Z_{eff} = 0.28\ A_{eff}^{(1.329 - 0.0471 \ln E)}.E^{0.092} \quad (7)$$

RESULTS AND DISCUSSION

The chemical compositions of the vitamins studied in the present work are given in table1.The vitamins listed C, B_3, B_1, B2, B9 and P have the same behavior since they consist of hydrogen, carbon and oxygen in about the same proportions. This is also evident from the fact that they all have a mean atomic number,‹Z›, of about 4.41(Table 1).The same arguments also hold for vitamins B_6, B_5 and A where ‹Z› is about 3.51.

Table1. Vitamins studied in the present work. ‹ Z › is the mean atomic number calculated from the chemical formula

Vitamins	‹Z ›	Vitamins	‹Z ›
VitaminC ($C_3H_4O_3$)	4.6	VitaminK ($C_{13}H_{16}CINO$)	5.09
VitaminB$_3$ ($C_6H_5NO_2$)	4.57	VitaminB$_2$ ($C_{17}H_{20}N_4O_6$)	4.21
VitaminB$_6$ ($C_8H_{12}N_2O_2$)	3.75	Vitamin D ($C_{27}H_{44}O$)	2.97
VitaminB$_5$ ($C_9H_{17}NO_5$)	3.69	Vitamin E ($C_{29}H_{50}O_2$)	2.96
Vitamin A ($C_{20}H_{30}O$)	3.1	VitaminB$_9$ ($C_{19}H_{19}N_7O_6$)	4.51
VitaminB$_1$ ($C_{12}H_{17}N_5O_4S$)	4.41	Vitamin P ($C_{28}H_{34}O_{15}$)	4.18

The total attenuation cross sections of the vitamins obtained from an accurate database of photon –interaction cross section are listed in table 2.

Table 2. Total attenuation cross sections (in barn/molecule) of vitamins

Compound	Formula	A	145.4 (keV)	279.2 (keV)	514 (keV)	661.6 (keV)	1115.5 (keV)	1173.2 (keV)	1332.1 (keV)
VitaminC	$C_3H_4O_3$	88.06	22.79	17.2	13.23	11.87	9.48	9.28	8.78
VitaminB$_3$	$C_6H_5NO_2$	123.11	31.87	24.04	18.49	16.59	13.25	12.97	12.28
VitaminB$_6$	$C_8H_{12}N_2O_2$	168.2	43.54	32.85	25.27	22.67	18.11	17.72	16.78
VitaminB$_5$	$C_9H_{17}NO_5$	219.24	56.75	42.82	32.93	29.55	23.6	23.1	21.87
Vitamin A	$C_{20}H_{30}O$	286.46	74.15	55.94	40.03	38.6	30.84	30.18	28.57
VitaminB$_1$	$C_{12}H_{17}N_5O_4S$	327.36	84.73	63.93	49.17	44.12	35.24	34.48	32.65
VitaminK	$C_{13}H_{16}CINO$	341.19	88.31	66.63	51.25	45.98	36.73	35.94	34.03
VitaminB$_2$	$C_{17}H_{20}N_4O_6$	376.37	97.42	73.5	56.54	50.72	40.52	39.65	37.54
Vitamin D	$C_{27}H_{44}O$	384.64	99.56	75.2	57.78	51.83	41.41	40.52	38.36
Vitamin E	$C_{29}H_{50}O_2$	430.71	111.35	84.11	64.7	58.04	46.37	45.37	42.96
VitaminB$_9$	$C_{19}H_{19}N_7O_6$	441.4	114.25	86.2	66.3	59.48	47.52	46.5	44.03
Vitamin P	$C_{28}H_{34}O_{15}$	610.56	158.04	119.24	91.71	82.28	65.73	64.32	60.9

The linear nature of the plots of total attenuation cross sections as a function of molecular weight is as shown in Figure 1.

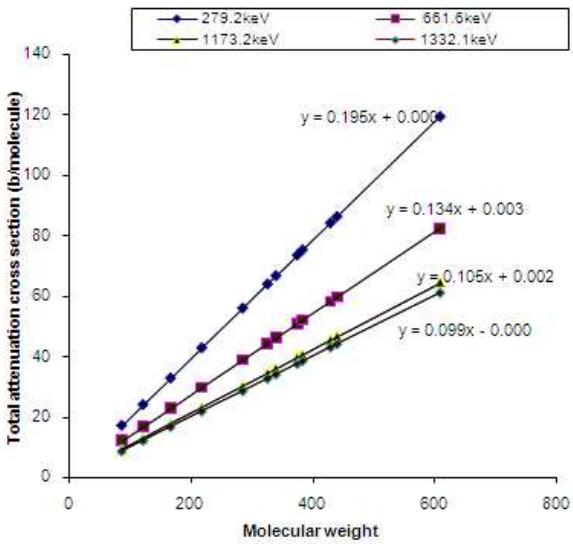

Figure 1. Total attenuation cross sections as a function of molecular weight

It is observed that the same value of total attenuation cross sections for all the compounds of the same molecular weight but different chemical structure at a given energy within the experimental errors [20-23] and the total attenuation cross section σ is linearly related to the molecular weight A and the energy E.

Plots of Z_{eff} values of the samples with respect to their effective atomic weights A_{eff} at energies 145.4, 279.2 and 1173.2keV are shown in Figures 2-5. The plots were found to be linear at each energy of interest E.

Further, it was worth noting from the values tabulated in table 3 in the energy region of present interest that the Z_{eff} values of the H, C, N and O samples used in the present work were related to their respective effective atomic weight through the relation

$$Z_{eff} = 0.533\ A_{eff}. \qquad (8)$$

The Z_{eff} values were used to calculate the electron densities of these samples. The values of Z_{eff} and N_e of these samples so obtained are tabulated in tables 3.Further, a quantity A_{eff} called the effective atomic weight was calculated as the molecular weight divided by the total number of atoms of all types present in the sample. Plots of Z_{eff} values of the samples with respect to their effective atomic weights A_{eff} at energies 145.4, 279.2 and 1173.2keV are shown in Figures 2-5. The plots were found to be linear at each energy of interest E.

Table 3. Effective atomic number Z_{eff} and electron density N_e (10^{24} electrons g^{-1}) of vitamins

Vitamins	A	145.4keV		279.2kev		514 keV		661.6keV		1115.5keV		1173.2keV		1332.1keV	
		Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e
VitaminC	88.06	4.79	0.328	4.76	0.326	4.73	0.324	4.71	0.322	4.69	0.321	4.68	0.320	4.68	0.320
VitaminB_3	123.11	4.78	0.328	4.75	0.326	4.72	0.324	4.70	0.322	4.68	0.321	4.67	0.321	4.66	0.319
VitaminB_6	168.20	3.73	0.321	3.73	0.321	3.73	0.321	3.73	0.321	3.73	0.321	3.73	0.321	3.73	0.321
VitaminB_5	219.24	3.64	0.320	3.64	0.320	3.64	0.320	3.65	0.321	3.65	0.321	3.65	0.321	3.65	0.321
Vitamin A	286.46	2.93	0.314	2.95	0.316	2.97	0.318	2.98	0.319	2.99	0.321	2.99	0.321	3.00	0.322
VitaminB_1	327.36	4.54	0.326	4.52	0.324	4.50	0.323	4.49	0.322	4.47	0.321	4.47	0.321	4.46	0.320
Vitamin K	341.19	5.71	0.333	5.64	0.329	5.58	0.325	5.55	0.324	5.50	0.321	5.49	0.320	5.48	0.319
VitaminB_2	376.37	4.31	0.325	4.30	0.323	4.28	0.322	4.27	0.321	4.26	0.321	4.26	0.321	4.25	0.320
Vitamin D	384.64	2.77	0.313	2.79	0.315	2.82	0.318	2.83	0.319	2.85	0.321	2.85	0.321	2.85	0.321
Vitamin E	430.71	2.76	0.312	2.78	0.315	2.80	0.318	2.81	0.319	2.83	0.321	2.83	0.321	2.84	0.322
VitaminB_9	441.40	4.70	0.327	4.67	0.325	4.64	0.323	4.63	0.322	4.61	0.321	4.60	0.321	4.59	0.320
Vitamin P	610.56	4.27	0.324	4.25	0.323	4.24	0.322	4.23	0.321	4.22	0.320	4.22	0.320	4.21	0.320

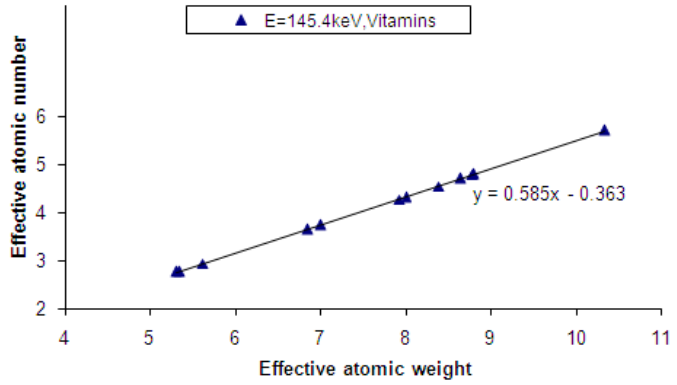

Figure 2. Effective atomic numbers of Vitamins as a function of Aeff at 145.4 keV

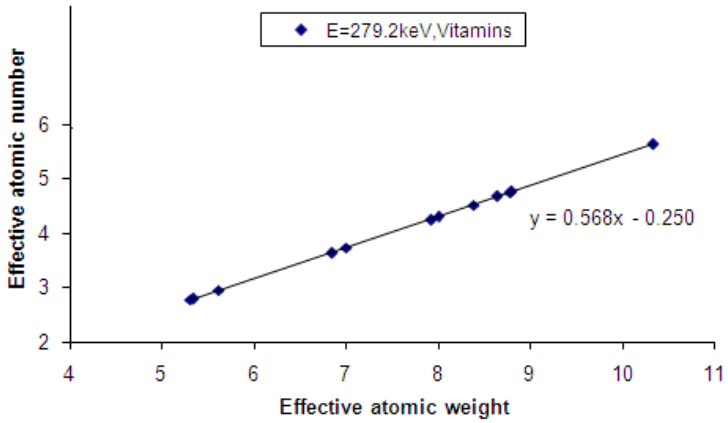

Figure 3. Effective atomic numbers of Vitamins as a function of Aeff at 279.2 keV

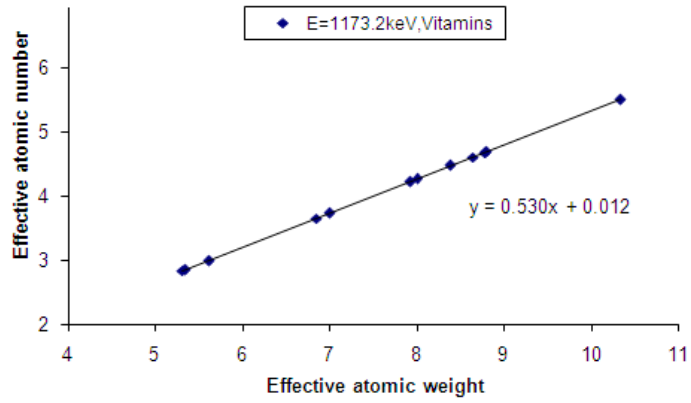

Figure 4. Effective atomic numbers of Vitamins as a function of Aeff at 1173.2 keV

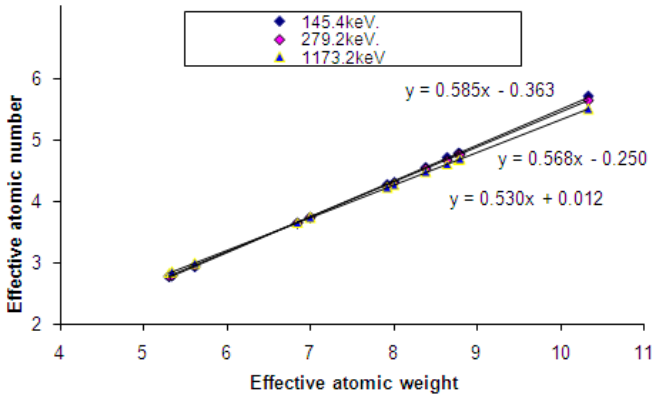

Figure 5. Effective atomic numbers of Vitamins as a function of Aeff at 145.4, 279.2keV and1173.2 keV

The present calculations are based on atomic photon–interaction cross sections. Therefore, Z_{eff} (and N_e) have the same value for compounds having the same chemical formula. In the present approximation, Z_{eff} and N_e are independent of any effects due to chemical bonding. A much larger and higher-dimensional database would be required to accommodate molecular and other matrix environments of the target atom [1].Careful experiments would be required to study any possible effect of chemical bonding on photon-interaction cross sections and effective atomic numbers of bio-molecules. Such studies should, however, stimulate further theoretical developments.

CONCLUSION

(1) The effective atomic number, Z_{eff} and the corresponding effective electron density N_e of some vitamins have been calculated in the energy region from 5-1500keV using WinXCom [1], and its underlying database of atomic photon-interaction cross sections [19].
(2) The ratio Z_{eff} / A_{eff} was 0.533 for vitamins containing H, C, N and O elements in the energy region 5-1500 keV then the value of effective atomic number of the samples containing H, C, N and O is almost a constant in the energy region 5-1500 keV.
(3) It has been observed that the same value of total attenuation cross sections for all the compounds of the same molecular weight but different chemical structure at a given energy.
(4) The conclusion of this work also confirms the results of our studies on other H, C, N and O based biomolecular system [24-26].

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