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Molar extinction coefficients of some proteins

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ABSTRACT

Mass attenuation coefficients (μ/ρ) and molar extinction coefficients (ε) of gamma rays in some proteins, viz. Actin-N($C_6H_6N_4O_4$), Collagen ($C_2H_5NOC_5H_9NOC_5H_{10}NO_2$), Serum Amyloid P Component ($C_{16}H_{24}N_2O_6$), Arp 2/3($C_{17}H_{16}BrNO_3S$), CFTR Inhibitor IV,PPQ-102 ($C_{26}H_{22}N_4O_3$),CFTR Inhibitor 11.Gly H-101($C_{19}H_{15}Br_2N_3O_3$),Elastin($C_{27}H_{48}N_6O_6$), C-reactive protein ($C_{62}H_{93}N_{13}O_{16}$), Myosin ($C_{60}H_{105}N_{23}O_{11}$), Serum albumin ($C_{2936}H_{4624}N_{786}O_{889}S_{41}$), have been calculated at the photon energies 123, 360, 511, 662, 1170, 1280 and 1330 keV.The effective atomic number and electron density have also been derived and the results are discussed.

Keywords: Mass attenuation coefficient, Atomic cross section, Proteins, Molar extinction coefficients, Effective atomic number and Electron density.

INTRODUCTION

The study of X-rays and gamma rays attenuation coefficient has received a great stimulus from the development of the radiation (X-ray and gamma ray) scanners and its application to medical diagnosis and treatment planning [1-3] .The fundamental physics of photon interactions with atoms is well understood and computational methods have advanced very significantly in recent years. Reliable data on the transmission and absorption of X-rays and gamma rays in biological, shielding and dosimetric materials are needed in medical physics and radiation biology as well as in many other fields. Ionizing radiation and radioactive materials play a major role as effective tools in the field of medicine, biological studies and industry.^{137}Cs (with photon energy 661.6 keV and ^{60}Co (with photon energy 1173 and 1332.5 keV) radio isotopes are being increasingly used in radiation therapy and oncology. The high energy of these isotopes along with optimal long life has increased the adaptability of these sources not only in the medical field but also in industry; biological studies and radiation sterilization [4] .Data on the total attenuation cross sections of proteins are quite useful. Especially since these are the building blocks which are essential to all living matter. We have theoretically obtained photon interaction cross section (σ_i)

mass attenuation coefficient (μ/ρ) molar extinction coefficients (ε) effective atomic number (Z_{eff}) and electron density N_e of several proteins for photons in the energy range 123-1330 keV of most interest in medical and biological application.

Theory

When a well –collimated narrow beam of gamma rays passing through a sample of thickness t composed of a single element of atomic number Z and assume that no scattered photons reach the collimated detector. The ratio of the intensity of X –rays emerging from the target along the incident direction to the incident intensity is given by

$$I/I_o = \exp(-\mu t) \qquad (1)$$

where μ is the linear attenuation coefficient of the target, which is related to the mean free path τ in the target and the atomic cross –section ${}_a\sigma$ by the expression

$$\mu = 1/\tau = n\, {}_a\sigma. \qquad (2)$$

The mass attenuation coefficient (μ/ρ) is given by

$$\mu/\rho = \frac{1}{\rho}\,\frac{\rho N_A}{A}\,{}_a\sigma \qquad (3)$$

where ρ is the density of the material, NA is Avogadro's number and A is the atomic weight. Thus for an idealized narrow –beam geometry, where the secondary radiations are not seen by the detector, the attenuation can be described by the well-known law:

$$\ln(I/I_o) = -\sigma Nx, \qquad (4)$$

where I_o is the incident intensity, I is the emergent intensity,σ is the total interaction cross section of the molecule, N is the number of molecules per unit volume, and x is the thickness of the slab. The product σ N is known as the linear attenuation coefficient μ.

The equation (4) can be rewritten in the following form known as Beer's law

$$\varepsilon = \frac{1}{\ln 10} N_A\sigma = \frac{1}{\ln 10} M\,\mu/\rho, \qquad (5)$$

where ε is the molar extinction coefficients, $\frac{1}{\ln 10} = 0.4343$, M is the Molar mass (g/mol).

In the present case atomic cross section σ_i have been obtained from mass attenuation coefficient μ/ρ using the following expression

$$\sigma_i = \frac{A_i\,(\mu/\rho)_i}{N_A}. \qquad (6)$$

Where Ai is the atomic mass of the constituent element i, N_A is the Avogadro's number whose value is 6.02486 $x10^{23}$.

The mass attenuation coefficients, μ/ρ, of proteins have been computed in the energy range 123 keV to 1330keV using a software programe [5].

Molar extinction coefficients ε have been calculated using equation (5) and atomic cross section σ_i have been obtained from equation (6), then effective electronic cross section ,

σ_{el} is calculated by equation (7)

$$\sigma_{el} = \sum fi\ \sigma_i / Z_i \qquad (7)$$

where Z_i is the atomic number of element i.

and finally effective atomic number Z_{eff} have been calculated using equation (8) [6].

$$Z_{eff} = 0.28\ A_{eff}^{\ (1.329-0.0471 \ln E)}\ E^{\ 0.092} \qquad (8)$$

Using these values of Z_{eff} electron density N_e can be calculated by using the expression (9) [7].

$$N_e = \frac{\mu/\rho}{\sigma_{el}} \qquad (9)$$

For a single element, the three γ-ray processes-photoelectric, Compton and pair production, can be expressed as a function of photon energy $h\nu$ and the atomic number Z of the element. At a given photon energy, the interaction is proportional to Z^n where n is between 4 and 5 for the photoelectric effect, 1 for the Compton effect, and 2 for pair production [8-10].For the purposes of γ-ray attenuation, a heterogeneous material, consisting of a number of elements in varying proportions, can be described as a fictitious element having an effective atomic number Z_{eff} .

The parameter Z_{eff} is very useful in choosing a substitute composite material in place of an element for that energy depending on the requirement. The energy absorption in the given medium can be calculated by means of well-established formulae if certain constants such as Z_{eff} and N_e of the medium are known. Among the parameters determining the constitutive structure of an unknown object or material, one should especially note the effective atomic number. In fact, this value can provide an initial estimation of the chemical composition of the material. A large Z_{eff} generally corresponds to inorganic compounds and metals. While a small Z_{eff} ($\leq$10) is an indicator of organic substances. Z_{eff} also finds its utilization in the computation of some other useful parameters, namely the absorbed dose and build-up factor.

In this paper we have therefore obtain the energy dependence of Z_{eff} and electron density N_e for different proteins. In the energy regime which is widely used in medical applications. There have been several reports on similar studies on different organic compounds [11-24] .

RESULTS AND DISCUSSION

The mass attenuation coefficients of gamma rays were obtained [23]for viz. Actin-N($C_6H_6N_4O_4$), Collagen ($C_2H_5NOC_5H_9NOC_5H_{10}NO_2$), Serum Amyloid P Component ($C_{16}H_{24}N_2O_6$), Arp 2/3($C_{17}H_{16}BrNO_3S$),CFTR InhibitorIV,PPQ-102($C_{26}H_{22}N_4O_3$),CFTR Inhibitor 11.Gly H-101($C_{19}H_{15}Br_2N_3O_3$),Elastin($C_{27}H_{48}N_6O_6$),

C-reactive protein ($C_{62}H_{93}N_{13}O_{16}$), Myosin ($C_{60}H_{105}N_{23}O_{11}$), Serum albumin ($C_{2936}H_{4624}N_{786}O_{889}S_{41}$at the photon energies 123, 360,511,662,1170,1280and 1330 keVusing XCOM programe. The values of mass attenuation coefficients thus determined are given in table1.The values of molar extinction coefficients ε are determined from equation (5).The results are shown in table 2. The energy dependence of the molar extinction coefficients for three proteins having molar mass 198.14, 493.15 and 66472.10 (g/mol) are shown graphically.

Figure1 shows the variation of molar extinction coefficients (ε) with energy for Actin-N. Figure1 essentially depicts the energy dependence of the Compton scattering cross section Compton Scattering is the main attenuation process contributing more than 99% to the total cross sections. The variation of molar extinction coefficients (ε) with energy for other two typical samples CFTR Inhibitor 11.Gly H-101 and Serum albumin also exhibits similar behaviour.as shown in Figure 2 and Figure3. Using the μ/ρ data for the element hydrogen, carbon, oxygen and nitrogen H, C, O and N, the electron density, N_e, have been determined from equation (9) and the results are given in table 3. It is observed that the values of N_e is almost constant, in the range 0.333-0.317*10 ^{24}.g^{-1}. It is observed that there is very small change in N_e with energy. Values of effective atomic number Z_{eff} of the proteins have also been determined from equation (8) and the results are given in table 4. For all proteins it is observed that the values of Z_{eff} lie in the range 5.47-3.35.

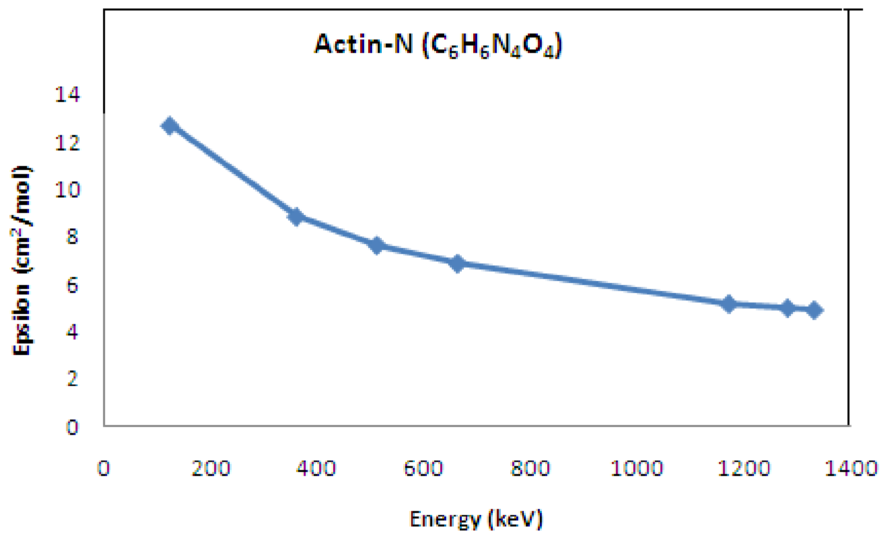

Fig 1. Molar extinction coefficient of Actin-N ($C_6H_6N_4O_4$).

Table 1. Mass attenuation coefficients μ/ρ (in cm^2/g)/molecule) of proteins

Compound	Formula	A	123 (keV)	360 (keV)	511 (keV)	662 (keV)	1170 (keV)	1280 (keV)	1330 (keV)
Actin-N	$C_6H_6N_4O_4$	198.14	0.148	0.103	0.089	0.080	0.060	0.058	0.057
Collagen	$C_2H_5NOC_5H_9NOC_5H_{10}NO_2$	273.34	0.154	0.108	0.093	0.084	0.063	0.061	0.059
Serum Amyloid P Component	$C_{16}H_{24}N_2O_6$	340.37	0.154	0.108	0.093	0.084	0.063	0.061	0.058
Arp 2/3	$C_{17}H_{16}BrNO_3S$	394.29	0.222	0.105	0.088	0.079	0.060	0.057	0.056
CFTR Inhibitor IV,PPQ-102	$C_{26}H_{22}N_4O_3$	438.49	0.150	0.106	0.091	0.082	0.062	0.059	0.058
CFTR Inhibitor 11.Gly H-101	$C_{19}H_{15}Br_2N_3O_3$	493.15	0.259	0.106	0.089	0.079	0.059	0.056	0.055
Elastin	$C_{27}H_{48}N_6O_6$	552.71	0.157	0.108	0.095	0.085	0.063	0.062	0.060
C-reactive protein	$C_{62}H_{93}N_{13}O_{16}$	1276.49	0.154	0.108	0.093	0.084	0.063	0.060	0.058
Myosin	$C_{60}H_{105}N_{23}O_{11}$	1324.64	0.155	0.109	0.094	0.082	0.065	0.062	0.059
Serum albumin	$C_{2936}H_{4624}N_{786}O_{889}S_{41}$	66472.10	0.154	0.107	0.093	0.084	0.063	0.061	0.058

Theoretical μ/ρ by XCOM program of Proteins.

Table 2 Molar extinction coefficients ε ($cm^2\ mol^{-1}$) of some Proteins

Sample	Molar mass (g/mol)	Molar extinction coefficients ε ($cm^2\ mol^{-1}$)						
		123 keV	360 keV	511 keV	662keV	1170 keV	1280 keV	1330 keV
Actin-N ($C_6H_6N_4O_4$)	198.14	12.736	8.863	7.659	6.884	5.163	4.991	4.905
Collagen ($C_2H_5NOC_5H_9NOC_5H_{10}NO_2$)	273.34	18.282	12.821	11.040	9.972	7.479	7.241	7.004
Serum Amyloid P Component ($C_{16}H_{24}N_2O_6$)	340.37	22.765	15.965	13.748	12.417	9.313	9.017	8.574
Arp 2/3 ($C_{17}H_{16}BrNO_3S$)	394.29	38.015	17.980	15.069	13.528	10.274	9.761	9.589
CFTR Inhibitor IV,PPQ-102 ($C_{26}H_{22}N_4O_3$)	438.49	28.565	20.186	17.330	15.616	11.807	11.236	11.045
CFTR Inhibitor 11.Gly H-101 ($C_{19}H_{15}Br_2N_3O_3$)	493.15	55.471	22.703	19.062	16.920	12.636	11.994	11.780
Elastin $C_{27}H_{48}N_6O_6$	552.71	37.687	25.925	22.804	20.404	15.123	14.883	14.403
C-reactive protein $C_{62}H_{93}N_{13}O_{16}$	1276.49	85.374	59.873	51.557	46.568	34.926	33.263	32.154
Myosin $C_{60}H_{105}N_{23}O_{11}$	1324.64	89.170	62.707	54.077	47.174	37.394	35.668	33.942
Serum albumin $C_{2936}H_{4624}N_{786}O_{889}S_{41}$	66472.10	4445.800	3088.965	2684.801	2424.982	1818.737	1760.999	1674.392

Table 3 Effective electron density, Ne, of some Proteins

Sample	Molar mass (g/mol)	Effective electron density, Ne (10^{24} g^{-1})						
		123 keV	360 keV	511 keV	662keV	1170 keV	1280 keV	1330 keV
Actin-N ($C_6H_6N_4O_4$)	198.14	0.333	0.327	0.325	0.324	0.319	0.321	0.319
Collagen ($C_2H_5NOC_5H_9NOC_5H_{10}NO_2$)	273.34	0.317	0.319	0.319	0.319	0.321	0.321	0.321
Serum Amyloid P Component ($C_{16}H_{24}N_2O_6$)	340.37	0.321	0.321	0.320	0.320	0.320	0.321	0.320
Arp 2/3 ($C_{17}H_{16}BrNO_3S$)	394.29	0.333	0.327	0.325	0.323	0.320	0.320	0.319
CFTR Inhibitor IV,PPQ-102 ($C_{26}H_{22}N_4O_3$)	438.49	0.325	0.323	0.322	0.321	0.320	0.320	0.320
CFTR Inhibitor 11.Gly H-101 ($C_{19}H_{15}Br_2N_3O_3$)	493.15	0.338	0.330	0.327	0.325	0.320	0.320	0.319
Elastin $C_{27}H_{48}N_6O_6$	552.71	0.318	0.320	0.320	0.320	0.321	0.321	0.321
C-reactive protein $C_{62}H_{93}N_{13}O_{16}$	1276.49	0.321	0.321	0.321	0.321	0.321	0.321	0.321
Myosin $C_{60}H_{105}N_{23}O_{11}$	1324.64	0.320	0.320	0.320	0.320	0.321	0.321	0.321
Serum albumin $C_{2936}H_{4624}N_{786}O_{889}S_{41}$	66472.10	0.322	0.321	0.321	0.321	0.321	0.321	0.320

Table 4 Effective atomic number, Z_{eff}, of some Proteins

Sample	Molar mass (g/mol)	Effective atomic number Z_{eff}						
		123 keV	360 keV	511 keV	662keV	1170 keV	1280 keV	1330 keV
Actin-N ($C_6H_6N_4O_4$)	198.14	5.47	5.38	5.34	5.32	5.26	5.27	5.25
Collagen ($C_2H_5NOC_5H_9NOC_5H_{10}NO_2$)	273.34	3.35	3..37	3.37	3.37	3.39	3.39	3.39
Serum Amyloid P Component ($C_{16}H_{24}N_2O_6$)	340.37	3.78	3..78	3.77	3.77	3.77	3.78	3.77
Arp 2/3 ($C_{17}H_{16}BrNO_3S$)	394.29	5.59	5.49	5.45	5.43	5.37	5.37	5.36
CFTR Inhibitor IV,PPQ-102 ($C_{26}H_{22}N_4O_3$)	438.49	4.30	4.28	4.26	4.25	4.24	4.24	4.23
CFTR Inhibitor 11.Gly H-101 ($C_{19}H_{15}Br_2N_3O_3$)	493.15	6.59	6.43	6.36	6.33	6.24	6.24	6.22
Elastin $C_{27}H_{48}N_6O_6$	552.71	3.35	3..37	3.37	3.37	3.38	3.39	3.39
C-reactive protein $C_{62}H_{93}N_{13}O_{16}$	1276.49	3.69	3..69	3.69	3.69	3.69	3.69	3.69
Myosin $C_{60}H_{105}N_{23}O_{11}$	1324.64	3.53	3..54	3.54	3.54	3.54	3.55	3.55
Serum albumin $C_{2936}H_{4624}N_{786}O_{889}S_{41}$	66472.10	3.83	3..82	3.82	3.82	3.82	3.82	3.81

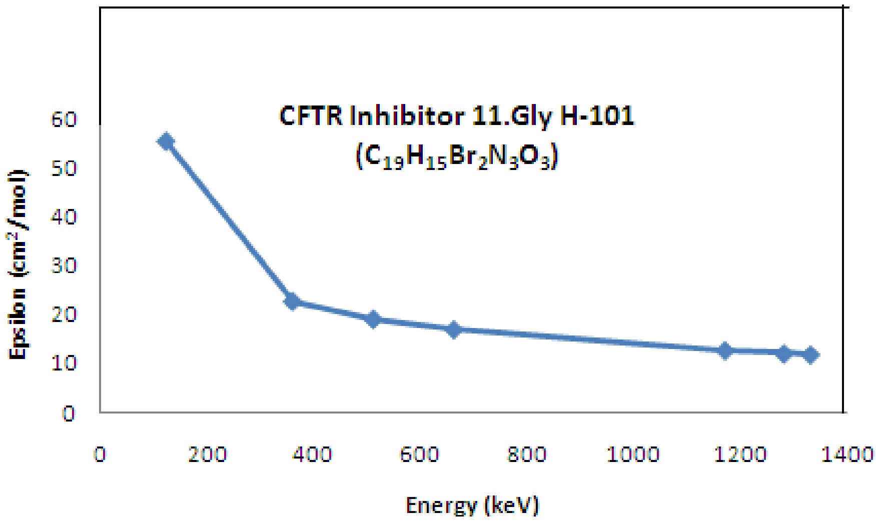

Fig 2. Molar extinction coefficient of CFTR Inhibitor 11.Gly H-101 ($C_{19}H_{15}Br_2N_3O_3$)

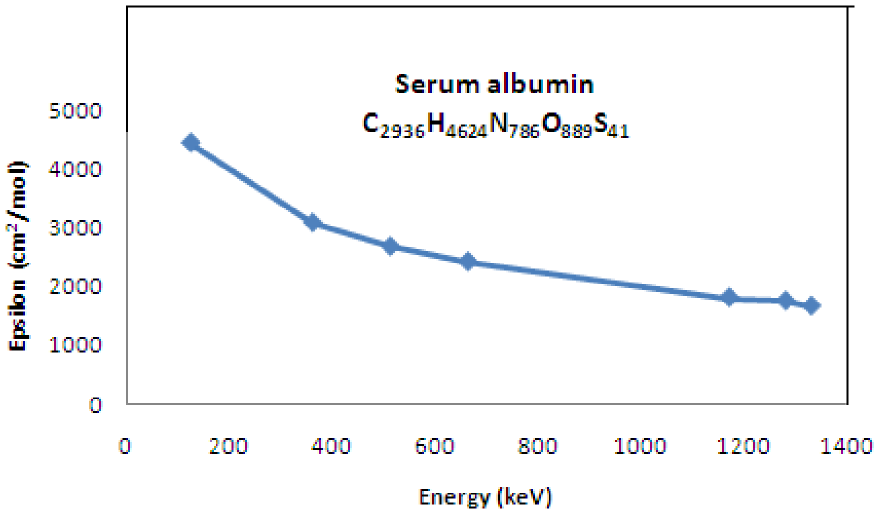

Fig 3. Molar extinction coefficient of Serum albumin $C_{2936}H_{4624}N_{786}O_{889}S_{41}$

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