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Molar extinction coefficients of some amino acids

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ABSTRACT

Mass attenuation coefficients(μ/ρ) *and molar extinction coefficients* (ε) *of gamma rays in some aminoacids,viz.Glycine*($C_2H_5NO_2$)*,Alanine*($C_3H_7NO_2$)*,Serine*($C_3H_7NO_3$)*,Proline* ($C_5H_9NO_2$)*, Valine* ($C_5H_{11}O_2N$)*, Isoleucine* ($C_6H_{13}NO_2$)*, Aspartic acid* ($C_4H_7NO_4$)*, Lysine* ($C_6H_{14}N_2O_2$)*, Glutamic acid* ($C_5H_9NO_4$)*, Asparagine* ($C_4H_8N_2O_3H_2O$)*, Histidine* ($C_6H_9N_3O_2$)*, Tyrosine* ($C_9H_{11}NO_3$)*, Tryptophan*($C_{11}H_{12}N_2O_2$) *and Cysteine*($C_6H_{12}N_2O_4S_2$)*,have been calculated at the photon energies 123, 360,511,662,1170,1280and 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, Amino acids, 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 amino acids are quite useful, especially since these are the building blocks of proteins 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 amino acids 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:

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

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 σN 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

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

Where Ai is the atomic mass of the constituent element i, N_A is the Avogadro's number whose value is 6.02486 $\times 10^{23}$.

The mass attenuation coefficients, μ/ρ, of amino acids 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)

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

where Z_i is the atomic number of element i.

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

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

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

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

For a single element, the three γ-ray processes-photoelectric, Compton and pair production, can be expressed as a function of photon energy hν 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} (≤ 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 amino acids. In the energy regime which is widely used in medical applications. There have been several reports on similar studies on different organic compounds [11-22] .

RESULTS AND DISCUSSION

The mass attenuation coefficients of gamma rays were obtained [23]for viz. Glycine ($C_2H_5NO_2$), Alanine ($C_3H_7NO_2$), Serine ($C_3H_7NO_3$), Proline ($C_5H_9NO_2$), Valine ($C_5H_{11}O_2N$), Isoleucine ($C_6H_{13}NO_2$), Asparticacid ($C_4H_7NO_4$), Lysine ($C_6H_{14}N_2O_2$), Glutamicacid ($C_5H_9NO_4$), Asparagine ($C_4H_8N_2O_3H_2O$), Histidine ($C_6H_9N_3O_2$), Tyrosine ($C_9H_{11}NO_3$), Tryptophan ($C_{11}H_{12}N_2O_2$) and Cysteine ($C_6H_{12}N_2O_4S_2$), at the photon energies 123, 360, 511, 662, 1170, 1280 and 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 amino acids having molar mass 75.1, 146.2 and 240.2 (g/mol) are shown graphically.

Table 1 Mass attenuation coefficient (μ/ρ) cm^2/g of Amino acids

Amino acids	123 keV	360 keV	511 keV	662 keV	1170 keV	1280 keV	1330 keV
1] Alanine $C_3H_7NO_2$	0.157	0.108	0.090	0.083	0.063	0.060	0.059
2]Asparagine $C_4H_8N_2O_3H_2O$	0.154	0.107	0.089	0.082	0.062	0.059	0.058
3]Aspartic acid $C_4H_7NO_4$	0.153	0.104	0.087	0.080	0.061	0.058	0.057
4] Cysteine $C_6H_{12}N_2O_4S_2$	0.161	0.105	0.087	0.080	0.060	0.058	0.056
5] Glutamic acid $C_5H_9NO_4$	0.154	0.105	0.088	0.081	0.062	0.059	0.057
6] Glycine $C_2H_5NO_2$	0.155	0.107	0.089	0.083	0.061	0.059	0.056
7] Histidine $C_6H_9N_3O_2$	0.154	0.106	0.088	0.082	0.061	0.059	0.055
8] Isoleucine $C_6H_{13}NO_2$	0.159	0.100	0.091	0.084	0.063	0.061	0.058
9] Lysine $C_6H_{14}N_2O_2$	0.159	0.100	0.091	0.083	0.063	0.061	0.058
10] Proline $C_5H_9NO_2$	0.156	0.108	0.089	0.083	0.062	0.060	0.057
11] Serine $C_3H_7NO_3$	0.155	0.106	0.089	0.082	0.061	0.059	0.056
12] Tryptophan $C_{11}H_{12}N_2O_2$	0.154	0.106	0.088	0.082	0.061	0.059	0.055
13] Tyrosine $C_9H_{11}NO_3$	0.154	0.106	0.088	0.082	0.061	0.059	0.056
14] Valine $C_5H_{11}O_2N$	0.158	0.110	0.091	0.084	0.064	0.061	0.057

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

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
Glycine ($C_2H_5NO_2$)	75.1	5.056	3.490	2.903	2.707	1.990	1.924	1.827
Alanine ($C_3H_7NO_2$)	89.1	6.075	4.177	3.483	3.212	2.438	2.322	2.283
Serine ($C_3H_7NO_3$)	105.1	7.075	4.838	4.062	3.743	2.784	2.693	2.556
Proline ($C_5H_9NO_2$)	115.1	7.798	5.399	4.449	4.149	3.099	2.999	2.849
Valine ($C_5H_{11}O_2N$)	117.1	8.035	5.594	4.628	4.272	3.255	3.102	2.899
Isoleucine ($C_6H_{13}NO_2$)	131.2	9.060	5.698	5.185	4.786	3.590	3.476	3.305
Aspartic acid ($C_4H_7NO_4$)	133.1	8.844	6.012	5.029	4.624	3.526	3.353	3.295
Lysine ($C_6H_{14}N_2O_2$)	146.2	10.096	6.350	5.778	5.270	4.000	3.873	3.683
Glutamic acid ($C_5H_9NO_4$)	147.1	9.838	6.708	5.622	5.175	3.961	3.769	3.642
Asparagine($C_4H_8N_2O_3H_2O$)	148.1	9.905	6.882	5.725	5.274	3.988	3.795	3.731
Histidine ($C_6H_9N_3O_2$)	155.2	10.380	7.145	5.932	5.527	4.112	3.977	3.707
Tyrosine ($C_9H_{11}NO_3$)	181.2	12.119	8.342	6.925	6.453	4.800	4.643	4.407
Tryptophan ($C_{11}H_{12}N_2O_2$)	204.2	13.657	9.401	7.804	7.272	5.410	5.232	4.878
Cysteine ($C_6H_{12}N_2O_4S_2$)	240.2	16.795	10.954	9.076	8.346	6.259	6.051	5.842

Table 3 Effective electron density, Ne, of some Amino acids

Sample	Molar mass (g/mol)	Effective electron density, Ne (10 ^{23} g^{-1})						
		123 keV	360 keV	511 keV	662keV	1170 keV	1280 keV	1330 keV
Glycine ($C_2H_5NO_2$)	75.1	4.04	3.99	3.97	3.96	3.93	3.92	3.92
Alanine ($C_3H_7NO_2$)	89.1	3.20	3.20	3.21	3.21	3.21	3.21	3.21
Serine ($C_3H_7NO_3$)	105.1	3.23	3.22	3.22	3.21	3.21	3.21	3.21
Proline ($C_5H_9NO_2$)	115.1	3.19	3.20	3.20	3.21	3.21	3.21	3.21
Valine ($C_5H_{11}O_2N$)	117.1	3.16	3.19	3.19	3.20	3.21	3.21	3.21
Isoleucine ($C_6H_{13}NO_2$)	131.2	3.15	3.18	3.19	3.20	3.21	3.21	3.21
Aspartic acid ($C_4H_7NO_4$)	133.1	3.26	3.24	3.23	3.22	3.21	3.20	3.20
Lysine ($C_6H_{14}N_2O_2$)	146.2	3.16	3.18	3.19	3.20	3.21	3.21	3.21
Glutamic acid ($C_5H_9NO_4$)	147.1	3.24	3.22	3.22	3.21	3.21	3.21	3.20
Asparagine($C_4H_8N_2O_3H_2O$)	148.1	3.22	3.22	3.21	3.21	3.21	3.21	3.21
Histidine ($C_6H_9N_3O_2$)	155.2	3.24	3.22	3.22	3.21	3.21	3.21	3.21
Tyrosine ($C_9H_{11}NO_3$)	181.2	3.23	3.22	3.22	3.21	3.21	3.21	3.21
Tryptophan ($C_{11}H_{12}N_2O_2$)	204.2	3.23	3.22	3.22	3.21	3.21	3.21	3.21
Cysteine ($C_6H_{12}N_2O_4S_2$)	240.2	3.30	3.25	3.24	3.23	3.20	3.20	3.20

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

Sample	Molar mass (g/mol)	Effective atomic number Z_{eff}						
		123 keV	360 keV	511 keV	662keV	1170 keV	1280 keV	1330 keV
Glycine ($C_2H_5NO_2$)	75.1	5.04	4.97	4.95	4.93	4.90	4.89	4.89
Alanine ($C_3H_7NO_2$)	89.1	3.64	3.64	3.65	3.65	3.65	3.65	3.65
Serine ($C_3H_7NO_3$)	105.1	4.02	4.01	4.01	4.00	4.00	4.00	4.00
Proline ($C_5H_9NO_2$)	115.1	3.59	3.60	3.60	3.60	3.61	3.61	3.61
Valine ($C_5H_{11}O_2N$)	117.1	3.24	3.26	3.27	3.27	3.28	3.29	3.29
Isoleucine ($C_6H_{13}NO_2$)	131.2	3.12	3.15	3.16	3.16	3.18	3.18	3.18
Aspartic acid ($C_4H_7NO_4$)	133.1	4.51	4.47	4.46	4.45	4.43	4.42	4.42
Lysine ($C_6H_{14}N_2O_2$)	146.2	3.20	3.22	3.23	3.23	3.25	3.25	3.25
Glutamic acid ($C_5H_9NO_4$)	147.1	4.16	4.14	4.14	4.13	4.12	4.12	4.12
Asparagine($C_4H_8N_2O_3H_2O$)	148.1	3.96	3.95	3.94	3.95	3.94	3.94	3.94
Histidine ($C_6H_9N_3O_2$)	155.2	4.17	4.15	4.15	4.14	4.13	4.13	4.13
Tyrosine ($C_9H_{11}NO_3$)	181.2	4.05	4.03	4.03	4.03	4.02	4.02	4.02
Tryptophan ($C_{11}H_{12}N_2O_2$)	204.2	4.05	4.04	4.04	4.03	4.03	4.02	4.02
Cysteine ($C_6H_{12}N_2O_4S_2$)	240.2	5.06	4.99	4.97	4.95	4.91	4.91	4.91

Figure1 shows the variation of molar extinction coefficients (ε) with energy for Glycine. 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 Lysine and Cysteine 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 4.04-3.15*10 ^{23}.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 amino acids have also been determined from equation (8) and the results are given in table 4. For all amino acids it is observed that the values of Z_{eff} lie in the range 5.04- 3.12.

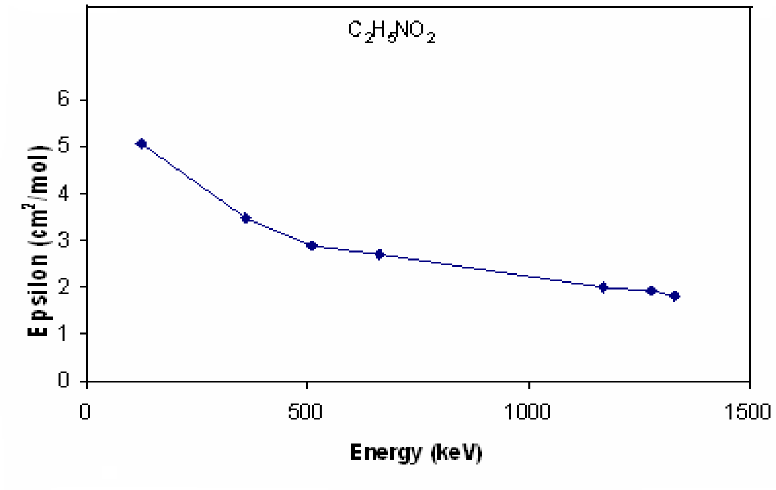

Fig 1. Molar extinction coefficient of $C_2H_5NO_2$.

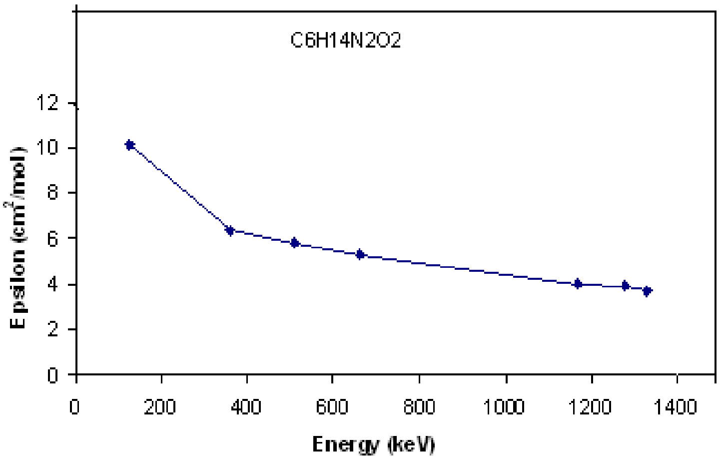

Fig 2. Molar extinction coefficient of $C_6H_{14}N_2O_2$

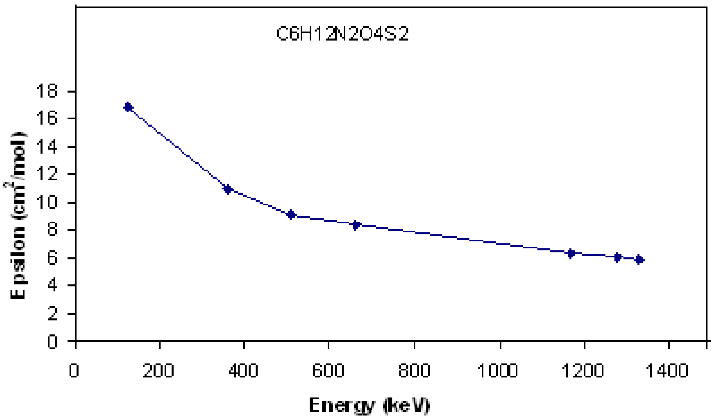

Fig 3. Molar extinction coefficient of $C_6H_{12}N_2O_4S_2$

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