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Study on gamma-ray attenuation characteristics of some amino acids for ^{133}Ba, ^{137}Cs, and ^{60}Co sources

Reza Bagheri[1] · **Ali Yousefi**[2] · **Seyed Pezhman Shirmardi**[3]

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Abstract Amino acids are the building blocks of proteins, which are the most abundant macromolecules in living cells. From the standpoint of the photon interaction cross sections of amino acids, the mass attenuation coefficients, half and tenth value layers, mean free path, effective atomic and electronic cross sections, effective atomic number, and effective electron density of fifteen essential amino acids have been determined for ^{133}Ba, ^{137}Cs, and ^{60}Co gamma-ray sources. The MCNP-4C code and the XCOM program have been used to calculate these parameters. The results have been compared to the available experimental and theoretical data. The theoretical results agreed with the experimental data, with RD values of $\leq \pm 7\%$. In the energy region of 81–1332.5 keV, it was found that the μ_m, σ_a, and σ_e values of the amino acids decreased as the photon energy increased, and the increasing density of amino acids had no steady effect on these quantities. Additionally, results demonstrated that the HVL, TVL, and MFP values increased with the increase in photon energy. The μ_m, σ_a, and Z_{eff} values of aspartic acid were the highest among those of all amino acids, and they were the lowest for isoleucine. The Z_{eff} value of each sample containing H, C, N, and O atoms was nearly constant in the studied energy region. The N_{eff} values of the studied amino acids varied in the range of 3.14×10^{23}–3.44×10^{23} electron/g. Furthermore, the N_{eff} values were approximately independent of the amino acid type in this energy region.

Keywords Amino acids · Mass attenuation coefficient · Effective electron density and atomic number · MCNP-4C · XCOM

1 Introduction

Proteins are vital molecules for every living organism. The DNA building blocks are made of proteins too. Amino acids are the building blocks of proteins [1], and there are 21 amino acids that are essential to the human body. Bearing in mind the vast application of X-ray and gamma-ray scanners in medical diagnostic and therapeutic methods [2], the increasing usage of industrial radioactive sources, like ^{60}Co and ^{137}Cs, for applications, such as labeling amino acids for imaging various tumors [3], it is valuable to evaluate gamma-ray attenuation characteristics of amino acids for these radioactive sources. Photons of the ^{133}Ba radionuclide in the energy range of 80–400 keV were found to be suitable for medical and biological applications, whereas ^{137}Cs and ^{60}Co radioisotopes are increasingly used in radiation therapy, oncology, industry, biological studies, and radiation sterilization [4].

There have been many studies on the interactions and effects of radiation on amino acids. In radiation sterilization, it is important to know the effect of radiation on proteins, amino acids, and their content in foods. Garrison [5] studied the various radiation-induced effects on amino

✉ Reza Bagheri
rzbagheri@aeoi.org.ir; reza_bagheri@aut.ac.ir

[1] Northwest Research Complex (Bonab), Radiation Applications Research School, Nuclear Science and Technology Research Institute, Tehran, Iran

[2] Materials and Nuclear Fuel Research School, Nuclear Science and Technology Research Institute, Tehran, Iran

[3] Radiation Applications Research School, Nuclear Science and Technology Research Institute, Tehran, Iran

acids, peptides, and proteins leading to amino acid degradation and to the synthesis of higher molecular weight amino acid derivatives. The effects of the radiation process on total protein and amino acid composition of raw and processed pearl millet flour during storage were described by Mohamed et al. [6]. Pawar and Bichile [7] measured the mass attenuation coefficient, effective atomic number, and electron density of six amino acids in the energy range of 0.122–1.330 MeV using a well-collimated narrow beam good geometry setup.

One of the best biomarkers of life that can survive in harsh environments like other planets and in space is amino acids. Hence, the radiation-amino acid interactions have been investigated by many researchers due to the exposure of amino acids to radiation in outer space. Kminek and Bada [8] studied the effect of ionizing radiation on the preservation of amino acids on Mars based on measured radiolysis constants of amino acids and radiation dose estimates. Furthermore, Cataldo et al. [9] studied solid-state radiolysis of amino acids with an astrochemical perspective, showing that the radiolysis rate constants of all the studied amino acids agreed with the radioracemization rate constant.

Additionally, the formation of free radicals in solid-state amino acids during exposure to radiation is a matter of concern in biological science and dosimetry. Foti et al. [10] investigated alanine amino acid decomposition induced by 200-keV helium and argon ion beams. A short description of produced radicals and an overview of the solid-state radiation chemistry of the simple amino acids were presented by Sagstuen et al. [11].

Furthermore, extensive theoretical and experimental studies of the radiation attenuation characteristics of various biological materials and organic compounds have been previously published. Mass attenuation coefficients of gamma rays in 48 mixtures and compounds of dosimetric interest were theoretically tabulated by Hubbell and Seltzer [12] in the energy range 1 keV to 20 MeV. Ermis et al. [13] calculated the gamma-ray mass attenuation coefficients of different parts of the human body using various theoretical methods, like FLUKA, GEANT4 Monte Carlo methods, and the XCOM program. Medhat et al. [14] calculated gamma-ray attenuation coefficients of some biological materials (blood, bones, and muscle) using Geant 4 and MCNP simulation codes and compared the obtained results with those obtained using XCOM and experimental data. Here, the mass attenuation coefficients, effective atomic numbers, and electron densities of six amino acids were calculated based on the methods described by Elbashir et al. [15], using MCNP5 simulations and XCOM program in the energy range 0.122–1.330 MeV. The linear attenuation coefficient of the breast tissue was experimentally determined by Tomal et al. [16]. Mass and linear attenuation coefficients of gamma rays for the glycine amino acid for 0.360, 0.662, 1.170, and 1.330 MeV photons were measured using Pawar and Mahajan [1]. Ahmadi et al. [17] obtained effective atomic numbers and electron densities of bacteriorhodopsin and its component amino acids in the energy range 1 keV–100 GeV using the WinXCom program. The attenuation parameters and energy absorption buildup factor of amine group materials in the energy range 122–1330 keV were experimentally calculated by Lokhande et al. [18] with the gamma-ray count in the narrow beam geometry condition. More et al. [19] experimentally determined the photon attenuation coefficients of *n*-acetyl-L-tryptophan, *n*-acetyl-L-tyrosine, D-tryptophan, *n*-acetyl-L-glutamic acid, D-phenylalanine, and D-threonine amino acids for ^{57}Co, ^{133}Ba, ^{137}Cs, ^{22}Na, ^{54}Mn, and ^{60}Co radioisotopes. The effective atomic numbers and electron densities of eight essential amino acids were calculated by Manohara and Hanagodimath [20] for total and partial photon interactions in the wide energy range of 1–100 GeV using the WinXCOM program.

Nair et al. [21, 22] experimentally measured total attenuation cross sections of sixteen amino acids for ^{133}Ba, ^{137}Cs, and ^{60}Co gamma-ray sources in a narrow beam good geometry setup. The effective atomic numbers and electron densities of the fifteen amino acids and eleven sugars were calculated by Gowda et al. [23] in the energy range 30–1333 keV using the measured total attenuation cross-section data reported by Nair et al. [21, 22]. In this article, a piecewise interpolation method was used to find the effective atomic numbers and electron densities of the compounds. In addition, a semiempirical formula was introduced using the logarithmic regression analysis of the XCOM data. Manjunathaguru and Umesh [24] calculated effective atomic numbers and electron densities of some biologically important compounds, like cholesterol, fatty acids, sugars, and some amino acids containing H, C, N, and O atoms in the energy range 145–1330 keV, using a new matrix method and a semiempirical relation for Z_{eff}. Additionally, they derived a semiempirical relation that can be used to determine the total attenuation cross sections of samples containing H, C, N, and O in the energy range 145–1332 keV based on the experimental total attenuation cross-section values of several sugars, amino acids, and fatty acids.

Here, fifteen amino acids, namely glycine, alanine, serine, valine, threonine, leucine, isoleucine, aspartic acid, lysine, glutamic acid, histidine, phenylalanine, arginine, tyrosine, and tryptophan, were considered for gamma-ray attenuation studies. The mass attenuation coefficients, half and tenth value layers, mean free path, effective atomic and electronic cross sections, effective atomic number, and effective electron density of these amino acids were

Table 1 Properties of amino acids

Amino acid	Chemical formula	Molecular weight (g mol^{-1})	Density (g cm^{-3})	Element			
				H	C	N	O
Glycine	$C_2H_5NO_2$	75.07	1.595	0.0671	0.3200	0.1866	0.4263
Alanine	$C_3H_7NO_2$	89.09	1.420	0.0792	0.4044	0.1572	0.3592
Serine	$C_3H_7NO_3$	105.09	1.600	0.0671	0.3429	0.1333	0.4567
Valine	$C_5H_{11}NO_2$	117.15	1.230	0.0946	0.5126	0.1196	0.2732
Threonine	$C_4H_9NO_3$	119.12	1.307	0.0762	0.4033	0.1176	0.4029
Leucine	$C_6H_{13}NO_2$	131.17	1.035	0.0999	0.5494	0.1068	0.2439
Isoleucine	$C_6H_{13}NO_2$	131.17	1.035	0.0999	0.5494	0.1068	0.2439
Aspartic acid	$C_4H_7NO_4$	133.10	1.514	0.0530	0.3609	0.1052	0.4808
Lysine	$C_6H_{14}N_2O_2$	146.19	1.125	0.0965	0.4930	0.1916	0.2189
Glutamic acid	$C_5H_9NO_4$	147.13	1.538	0.0617	0.4082	0.0952	0.4350
Histidine	$C_6H_9N_3O_2$	155.15	1.423	0.0585	0.4645	0.2708	0.2062
Phenyl alanine	$C_9H_{11}NO_2$	165.19	1.201	0.0671	0.6544	0.0848	0.1937
Arginine	$C_6H_{14}N_4O_2$	174.20	1.460	0.0810	0.4137	0.3216	0.1837
Tyrosine	$C_9H_{11}NO_3$	181.19	1.340	0.0612	0.5966	0.0773	0.2649
Tryptophan	$C_{11}H_{12}N_2O_2$	204.23	1.340	0.0592	0.6469	0.1372	0.1567

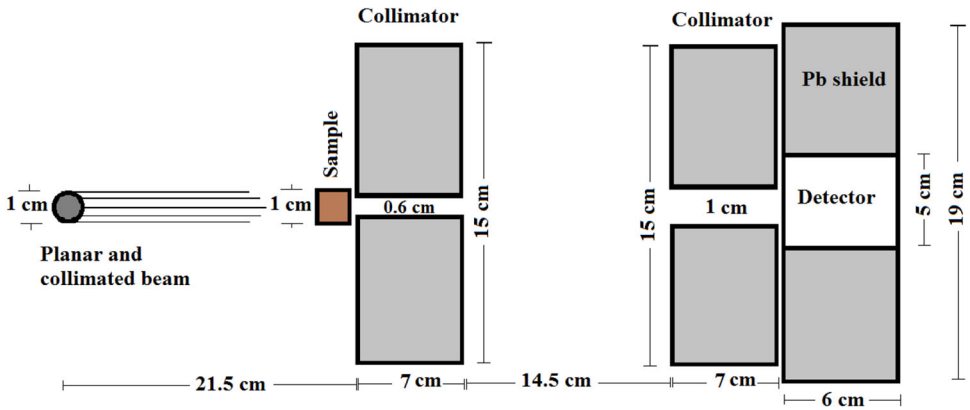

Fig. 1 Geometry of modeled configuration (sizes are not in scale)

calculated for ^{133}Ba (81, 276, 302.9, 356, and 383.9 keV), ^{137}Cs (661.6), and ^{60}Co (1173 and 1332.5 keV) gamma-ray sources using the MCNP-4C code and XCOM program for the first time. We tabulated obtained quantities and interpreted simulated and calculated results in terms of numerical values. Additionally, we verified and validated the MCNP-4C code and XCOM program with the available experimental and theoretical data. For this, the experimentally measured total attenuation cross sections determined by Nair et al. [21, 22], the semiempirical formula described by Manjunathaguru and Umesh [24] for the total attenuation cross sections of samples containing H, C, N, and O, the semiempirical formula described by Gowda et al. [23] for the calculation of Z_{eff} using a piecewise interpolation method, and finally the theoretical values obtained from the XAAMDI database (NIST physical reference data) and other experimental works were used.

The MCNP code is a general-purpose Monte Carlo radiation transport code, which models the interaction of radiation with matter [25]. Besides, the theoretical values for mass attenuation coefficients of different elements, compounds, and mixtures over a wide photon energy range were tabulated by Hubbell and Seltzer [12]. Using these tables and the computerized program WinXCom or its predecessor, XCOM program, mass attenuation coefficients were calculated at energies 1 keV to 100 GeV [26, 27].

Table 2 Mass attenuation coefficients ($\mu_m \times 10^{-2}$ cm^2 g^{-1}) of amino acids

Amino acid	Density (g cm^{-3})	Energy (keV)											
		81			276			302.9			356		
		A	B	C	A	B	C	A	B	C	A	B	C
Leucine	1.035	0.181	0.177	0.175	0.123	0.121	0.117	0.119	0.117	0.114	0.112	0.110	0.110
Isoleucine	1.035	0.181	0.177	0.174	0.123	0.121	0.117	0.119	0.117	0.111	0.112	0.110	0.108
Lysine	1.125	0.180	0.177	0.174	0.123	0.121	0.123	0.119	0.116	0.115	0.112	0.110	0.107
Phenyl alanine	1.201	0.176	0.172	0.174	0.119	0.117	0.115	0.115	0.113	0.112	0.109	0.107	0.105
Valine	1.230	0.181	0.177	0.174	0.122	0.120	0.118	0.118	0.116	0.112	0.112	0.109	0.106
Threonine	1.307	0.179	0.175	0.174	0.120	0.118	0.115	0.117	0.114	0.111	0.110	0.108	0.105
Tyrosine	1.340	0.176	0.172	0.174	0.119	0.117	0.115	0.115	0.113	0.111	0.108	0.106	0.106
Tryptophan	1.340	0.174	0.171	0.171	0.119	0.116	0.115	0.115	0.113	0.111	0.109	0.106	0.105
Alanine	1.420	0.179	0.175	0.174	0.121	0.119	0.119	0.117	0.115	0.114	0.110	0.108	0.107
Histidine	1.423	0.176	0.171	0.174	0.119	0.116	0.115	0.115	0.113	0.111	0.108	0.106	0.105
Arginine	1.460	0.179	0.175	0.174	0.121	0.119	0.115	0.117	0.115	0.114	0.110	0.108	0.105
Aspartic acid	1.514	0.176	0.172	0.174	0.118	0.116	0.115	0.115	0.112	0.111	0.107	0.105	0.105
Glutamic acid	1.538	0.176	0.173	0.174	0.119	0.117	0.115	0.115	0.113	0.111	0.109	0.106	0.105
Glycine	1.595	0.179	0.174	0.174	0.120	0.117	0.115	0.117	0.113	0.112	0.110	0.107	0.105
Serine	1.600	0.178	0.174	0.174	0.120	0.117	0.115	0.116	0.113	0.111	0.109	0.107	0.105
Amino acid	Density (g cm^{-3})	Energy (keV)											
		383.9			661.6			1173			1332.5		
		A	B	C	A	B	C	A	B	C	A	B	C
Leucine	1.035	0.109	0.107	0.106	0.087	0.085	0.084	0.067	0.065	0.065	0.062	0.060	0.061
Isoleucine	1.035	0.109	0.107	0.107	0.087	0.085	0.082	0.067	0.065	0.064	0.062	0.060	0.061
Lysine	1.125	0.108	0.106	0.103	0.086	0.085	0.082	0.066	0.064	0.064	0.062	0.060	0.061
Phenyl alanine	1.201	0.106	0.104	0.102	0.084	0.082	0.082	0.065	0.063	0.064	0.060	0.059	0.061
Valine	1.230	0.108	0.106	0.102	0.086	0.084	0.083	0.066	0.064	0.064	0.062	0.060	0.060
Threonine	1.307	0.106	0.104	0.105	0.085	0.083	0.082	0.065	0.063	0.064	0.061	0.059	0.060
Tyrosine	1.340	0.105	0.103	0.102	0.084	0.082	0.082	0.064	0.062	0.063	0.060	0.058	0.060
Tryptophan	1.340	0.105	0.103	0.102	0.083	0.082	0.082	0.064	0.062	0.063	0.060	0.058	0.059
Alanine	1.420	0.106	0.105	0.102	0.085	0.083	0.083	0.065	0.063	0.064	0.061	0.059	0.060
Histidine	1.423	0.105	0.103	0.102	0.083	0.082	0.082	0.064	0.062	0.064	0.060	0.058	0.059
Arginine	1.460	0.107	0.105	0.102	0.085	0.083	0.082	0.065	0.064	0.064	0.061	0.059	0.061
Aspartic acid	1.514	0.104	0.102	0.102	0.083	0.081	0.082	0.064	0.062	0.064	0.060	0.058	0.059
Glutamic acid	1.538	0.105	0.103	0.102	0.084	0.082	0.082	0.064	0.062	0.064	0.060	0.058	0.060
Glycine	1.595	0.106	0.104	0.103	0.085	0.082	0.082	0.065	0.063	0.063	0.061	0.059	0.059
Serine	1.600	0.106	0.104	0.102	0.084	0.082	0.082	0.064	0.063	0.064	0.061	0.059	0.060

A: MCNP-4C, B: XCOM, and C: experimental values [21, 22]

2 Materials and methods

2.1 Simulation

Cylindrical geometry was used for modeling amino acid samples. According to experimental conditions [21, 22], a cylinder of Φ1 cm and different thicknesses was defined for each amino acid sample. The thicknesses of the samples have not been mentioned in previous experimental studies [21, 22], and it has only been noted that the thickness of the samples was chosen such that a $\mu t < 0.4$ criterion was satisfied at each energy to minimize the effects of multiple scattering. Thus, the thickness was set to achieve the average value for each sample (μt was considered about 0.2). It should be noted that the thickness of the samples affects the shielding data analysis. When thick samples are

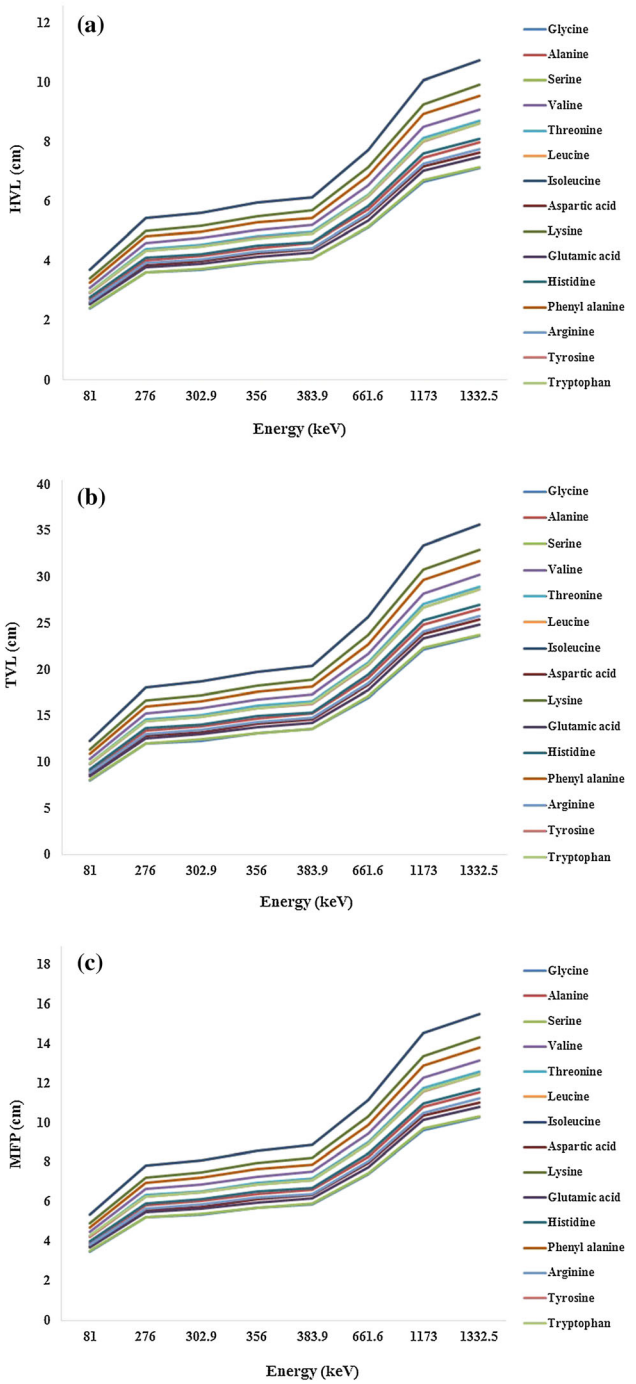

Fig. 2 (Color online) HVL (**a**), TVL (**b**), and MFP (**c**) values of amino acids obtained using the MCNP-4C code

used, these cause the incident photons to be scattered. These photons can reach the detector and render an overestimation of the transmitted intensity, resulting in an underestimation of the measured attenuation coefficients.

The attenuation coefficients were measured in narrow beam transmission geometry using sources, such as planar, collimated, and monoenergetic beams that emit gamma rays perpendicular to the front face of samples. A disk source of Φ1 cm and parallel to the surface of the samples was defined in a data card of MCNP code with ERG, PAR, POS, and DIR commands for energy, type of particle, position, and direction, respectively. The chemical formulas, elemental compositions, densities, and molecular weights of amino acids used in the material card of MCNP code are presented in Table 1.

A small cylinder of Φ5 cm $\times$ 6 cm was considered as the detector volume (an ORTEC HPGe detector model 23210 with Φ52.5 mm $\times$ 58.1 mm cylinder crystal was used in experiment). A Φ19 cm $\times$ 6 cm lead cylinder with a Φ1 cm $\times$ 6 cm hole was used as the detector shield and set behind a Φ1-cm lead collimator. Additionally, a Φ15 cm $\times$ 7 cm lead cylinder with a Φ0.6 cm $\times$ 7 cm hole was inserted between the samples and detector collimator. The geometry of the system is shown in Fig. 1, according to the experimental condition.

Tally F4 was used to obtain MCNP-4C simulated data. It calculates the average flux in a cell (detector volume) for only one incident gamma photon.

The simulations were performed with 100,000 histories. All simulated results were reported with a $\leq$ 0.5% error.

2.2 Theory

Linear and mass attenuation coefficients of samples (μ and μ_m) were derived using the transmission factors for various thicknesses of samples, using Lambert's law, which is described as follows [28]:

$$I = I_0 e^{-\mu t}, \tag{1}$$

where I_0 and I denote the intensities of photons incoming and outgoing through the attenuator, t is sample thickness, and μ denotes the linear attenuation coefficient. The mass attenuation coefficients were calculated by dividing the linear attenuation coefficient of each amino acid by its density.

On the contrary, the mass attenuation coefficients of glass samples were calculated using XCOM program data using Eq. (2), in which w_i and $\mu_{m,i}$ (obtained directly from the XCOM program) are the fractional weight and mass attenuation coefficient of the ith element in the sample, respectively [29]:

$$\mu_m = \sum_{i=1}^{n} w_i \times \mu_{m,i}. \tag{2}$$

Additionally, the HVL and TVL quantities are defined as the extent of attenuator thickness, which reduce photon intensity to half and tenth of its initial value, respectively. These quantities can be calculated using the following relations [4]:

Table 3 Effective atomic cross sections (barn/atom) of amino acids

Amino acid	Energy (keV)															
	81				276				302.9				356			
	A	B	C	D	A	B	C	D	A	B	C	D	A	B	C	D
Leucine	1.789	1.753	1.732	–	1.217	1.196	1.155	1.170	1.178	1.156	1.132	1.124	1.113	1.087	1.089	1.049
Isoleucine	1.789	1.753	1.723	–	1.217	1.196	1.155	1.170	1.178	1.156	1.103	1.124	1.113	1.087	1.073	1.049
Lysine	1.823	1.787	1.758	–	1.241	1.219	1.247	1.195	1.201	1.177	1.167	1.149	1.131	1.107	1.079	1.072
Phenyl alanine	2.102	2.050	2.074	–	1.425	1.399	1.371	1.410	1.377	1.351	1.330	1.354	1.299	1.271	1.257	1.263
Valine	1.854	1.808	1.779	–	1.252	1.232	1.205	1.210	1.209	1.190	1.147	1.163	1.142	1.119	1.089	1.085
Threonine	2.083	2.033	2.024	–	1.400	1.376	1.338	1.375	1.360	1.331	1.295	1.321	1.274	1.251	1.225	1.233
Tyrosine	2.207	2.150	2.183	–	1.494	1.463	1.442	1.482	1.443	1.413	1.396	1.424	1.357	1.329	1.325	1.328
Tryptophan	2.185	2.143	2.148	–	1.496	1.462	1.445	1.484	1.444	1.413	1.400	1.426	1.363	1.329	1.324	1.331
Alanine	2.036	1.991	1.977	–	1.374	1.351	1.355	1.345	1.328	1.305	1.298	1.292	1.255	1.227	1.215	1.206
Histidine	2.264	2.205	2.242	–	1.527	1.499	1.482	1.523	1.478	1.449	1.435	1.463	1.389	1.363	1.358	1.365
Arginine	1.993	1.941	1.936	–	1.343	1.322	1.279	1.315	1.301	1.277	1.265	1.263	1.226	1.202	1.173	1.179
Aspartic acid	2.430	2.373	2.403	–	1.637	1.601	1.588	1.633	1.584	1.547	1.538	1.569	1.481	1.455	1.456	1.463
Glutamic acid	2.263	2.221	2.237	–	1.529	1.502	1.479	1.520	1.477	1.450	1.432	1.460	1.400	1.364	1.355	1.362
Glycine	2.237	2.165	2.170	–	1.498	1.463	1.434	1.473	1.459	1.413	1.400	1.416	1.370	1.330	1.314	1.321
Serine	2.221	2.166	2.169	–	1.494	1.463	1.434	1.473	1.441	1.413	1.389	1.415	1.363	1.330	1.314	1.321
Amino acid	Energy (keV)															
	383.9				661.6				1173				1332.5			
	A	B	C	D	A	B	C	D	A	B	C	D	A	B	C	D
Leucine	1.078	1.055	1.051	1.015	0.857	0.840	0.830	0.804	0.659	0.639	0.640	0.628	0.617	0.599	0.600	0.595
Isoleucine	1.078	1.055	1.060	1.015	0.857	0.840	0.814	0.804	0.659	0.639	0.634	0.628	0.617	0.599	0.599	0.595
Lysine	1.093	1.075	1.044	1.037	0.872	0.855	0.829	0.821	0.672	0.651	0.648	0.642	0.628	0.610	0.613	0.607
Phenyl alanine	1.262	1.234	1.222	1.223	1.004	0.981	0.978	0.968	0.769	0.748	0.763	0.757	0.720	0.700	0.722	0.716
Valine	1.106	1.086	1.047	1.050	0.883	0.864	0.853	0.831	0.678	0.658	0.655	0.650	0.634	0.616	0.616	0.615
Threonine	1.239	1.215	1.221	1.193	0.989	0.966	0.953	0.944	0.757	0.736	0.745	0.738	0.708	0.689	0.703	0.699
Tyrosine	1.319	1.290	1.283	1.286	1.049	1.026	1.028	1.017	0.807	0.782	0.794	0.795	0.752	0.732	0.750	0.753
Tryptophan	1.319	1.290	1.287	1.288	1.048	1.026	1.030	1.019	0.806	0.782	0.789	0.797	0.753	0.732	0.741	0.754
Alanine	1.208	1.191	1.158	1.167	0.967	0.947	0.941	0.924	0.743	0.721	0.731	0.722	0.695	0.676	0.681	0.683
Histidine	1.353	1.323	1.315	1.321	1.073	1.052	1.057	1.045	0.824	0.801	0.825	0.817	0.772	0.750	0.760	0.774
Arginine	1.188	1.166	1.139	1.141	0.946	0.927	0.912	0.903	0.726	0.706	0.712	0.706	0.680	0.662	0.673	0.668
Aspartic acid	1.438	1.412	1.413	1.417	1.145	1.122	1.131	1.121	0.881	0.855	0.878	0.876	0.827	0.801	0.816	0.830
Glutamic acid	1.355	1.324	1.316	1.319	1.080	1.053	1.053	1.044	0.824	0.802	0.823	0.816	0.774	0.751	0.768	0.772
Glycine	1.327	1.290	1.280	1.278	1.059	1.026	1.022	1.012	0.811	0.782	0.788	0.791	0.762	0.732	0.734	0.749
Serine	1.316	1.290	1.276	1.278	1.047	1.026	1.022	1.012	0.803	0.782	0.798	0.791	0.755	0.732	0.754	0.749

A: MCNP-4C, B: XCOM, C: experimental [21, 22], and D: Manjunathaguru and Umesh values [24]

$$\mathrm{HVL} = \frac{\ln 2}{\mu}, \tag{3}$$

$$\mathrm{TVL} = \frac{\ln 10}{\mu}. \tag{4}$$

The interactions of gamma rays can also be analyzed using their mean free path, which is defined as the average distance travelled by the rays in the absorber before an interaction takes place [4]. The mean free path can be obtained as follows:

$$\mathrm{MFP} = \frac{1}{\mu}. \tag{5}$$

The total molecular cross sections (σ_t) of amino acids are calculated using the simulated and theoretical values of μ_m using the following relationship [23]:

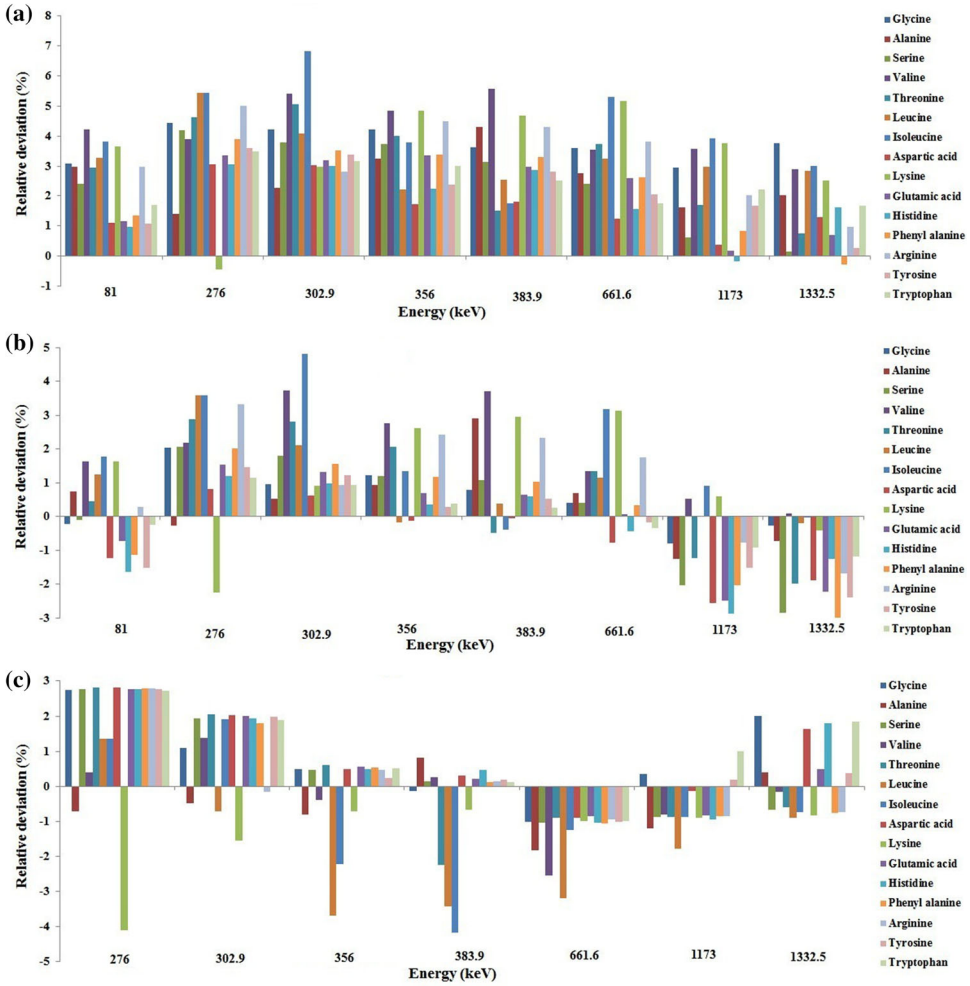

Fig. 3 (Color online) Difference (%) between experimental data and data obtained using **a** MCNP-4C, **b** XCOM, and **c** the semiempirical formula given by Manjunathaguru and Umesh [24]

$$\sigma_t = \frac{\mu_m M}{N_A}, \tag{6}$$

where M is the molecular weight of materials and N_A is Avogadro's number. The experimental values of the total molecular cross sections for amino acids were directly derived from Nair et al. [21, 22].

Additionally, the effective atomic and electronic cross sections (σ_a and σ_e) were calculated from the following mixture equations using the XCOM program and obtained total molecular cross sections [30–32]:

$$\sigma_a = \frac{1}{N_A}\sum f_i A_i \mu_{m,i} = \frac{\sigma_t}{\sum_i n_i}, \tag{7}$$

$$\sigma_e = \frac{1}{N_A}\sum \frac{f_i A_i \mu_{m,i}}{Z_i}, \tag{8}$$

where f_i denotes the fractional abundance of the ith element with respect to the number of atoms, such that $f_1 + f_2 + f_3 + \cdots + f_i = 1$, and Z_i and A_i are the atomic number and atomic weight of the ith element, respectively. Additionally, n_i is the atomic number of ith element in the material.

Finally, the effective atomic number (Z_{eff}) and effective electron density (N_{eff}) of samples are calculated using μ_m, σ_a, and, σ_e values and the following formulas [33]:

$$Z_{eff} = \frac{\sigma_a}{\sigma_e}, \tag{9}$$

$$N_{eff} = \frac{N_A Z_{eff}}{\sum f_i A_i} = \frac{\mu_m}{\sigma_e}. \tag{10}$$

3 Results and discussion

3.1 Mass attenuation coefficients HVL, TVL, and MFP of amino acids

The simulated and calculated values of mass attenuation coefficients (μ_m) compared to experimental data [21, 22] are given in Table 2 for the studied gamma-ray energies.

Table 4 Effective electronic cross sections (barn/electron) of amino acids

Amino acid	Density (g cm^{-3})	Molecular weight (g mol^{-1})	Energy (keV)							
			81	276	302.9	356	383.9	661.6	1173	1332.5
Leucine	1.035	131.17	0.5254	0.3649	0.3528	0.3319	0.3223	0.2565	0.1954	0.1830
Isoleucine	1.035	131.17	0.5254	0.3649	0.3528	0.3319	0.3223	0.2565	0.1954	0.1830
Lysine	1.125	146.19	0.5257	0.3649	0.3528	0.3319	0.3223	0.2565	0.1954	0.1830
Phenyl alanine	1.201	165.19	0.5272	0.3651	0.3529	0.3319	0.3223	0.2565	0.1954	0.1830
Valine	1.230	117.15	0.5260	0.3650	0.3528	0.3319	0.3223	0.2565	0.1954	0.1830
Threonine	1.307	119.12	0.5284	0.3651	0.3529	0.3320	0.3223	0.2565	0.1954	0.1830
Tyrosine	1.340	181.19	0.5284	0.3650	0.3529	0.3319	0.3223	0.2565	0.1954	0.1830
Tryptophan	1.340	204.23	0.5278	0.3650	0.3529	0.3319	0.3223	0.2565	0.1954	0.1830
Alanine	1.420	89.09	0.5279	0.3651	0.3529	0.3320	0.3223	0.2565	0.1954	0.1830
Histidine	1.423	155.15	0.5290	0.3651	0.3530	0.3320	0.3224	0.2565	0.1954	0.1830
Arginine	1.460	174.20	0.5270	0.3650	0.3529	0.3319	0.3223	0.2565	0.1954	0.1830
Aspartic acid	1.514	133.10	0.5316	0.3652	0.3531	0.3321	0.3224	0.2565	0.1954	0.1830
Glutamic acid	1.538	147.13	0.5301	0.3652	0.3530	0.3320	0.3224	0.2565	0.1954	0.1830
Glycine	1.595	75.07	0.5298	0.3651	0.3530	0.3320	0.3224	0.2565	0.1954	0.1830
Serine	1.600	105.09	0.5299	0.3651	0.3530	0.3320	0.3224	0.2565	0.1954	0.1830

The HVL, TVL, and MFP values were determined using Eqs. (3), (4), and (5), respectively. The dependencies of the HVL, TVL, and MFP of the amino acids on gamma-ray energy are demonstrated in Fig. 2.

As shown in Table 2, a good agreement was observed between experimental, simulated, and calculated values of μ_m. The discrepancies are considered and acceptable. It should be noted that the reported experimental errors were to the extent of $\pm$ 2% [21, 22].

As illustrated in Fig. 2, the HVL, TVL, and MFP values of the amino acids increase with the increase in photon energy and decreased with the increase in the density of amino acids. Additionally, it is obvious from Fig. 2 that isoleucine and serine, with the minimum and maximum amount of density, respectively, have the highest and lowest values of HVL, TVL, and MFP, respectively.

3.2 Effective atomic and electronic cross sections of amino acids

The MCNP-4C, XCOM, and experimental values of effective atomic cross sections of amino acids were calculated using Eqs. (6) and (7). Additionally, we calculated effective atomic cross sections of amino acids using the semiempirical formula given by Manjunathaguru and Umesh [24] for the total attenuation cross sections of samples containing H, C, N, and O in the energy range of 145–1330 keV. This formula relates total attenuation cross section (σ_t) to the molecular weight (M) and energy (E) as follows:

$$\sigma_t = 2.2ME^{-0.43}. \quad (11)$$

Table 3 shows the simulated, calculated, and experimental values of effective atomic cross sections.

The relative deviation (RD) differences between simulated and calculated results with the experimental data of effective atomic cross sections are plotted in Fig. 3 for MCNP-4C code, XCOM program, and semiempirical formula of Manjunathaguru and Umesh [24] using Eq. (12):

$$\mathrm{RD} = \{\mathrm{Theoretical} - \mathrm{Experimental}\} \times 100/\mathrm{Experimental}. \quad (12)$$

For all of the amino acids, the RD values ranged from $-$ 0.44 to 6.83%, $-$ 2.99 to 4.82%, and $-$ 4.17 to 2.81% for data obtained using MCNP-4C, XCOM, and the semiempirical formula given by Manjunathaguru and Umesh [24], respectively (see Fig. 3). The RD values were found to be $\leq \pm$ 7% for all amino acids. Additionally, it was found that the RD values were approximately independent of amino acid type, gamma-ray energy, and the σ_a calculation method.

Additionally, a good agreement was observed between experimental and theoretical values of σ_a. Tables 2 and 3 indicate that the μ_m and σ_a values of the amino acids decrease with the increase in the photon energy, while an increase in the density of amino acids does not monotonously increase these quantities.

It is obvious from Tables 2 and 3 that aspartic acid and isoleucine have the greatest and lowest values of μ_m and σ_a, respectively. The XCOM results showed better agreement with the experimental data than the MCNP-4C results.

Table 5 Effective atomic numbers (Z_{eff}) of amino acids

Amino acid	Energy (keV)											
	81						276					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	3.404	3.337	3.296	3.313	–	–	3.336	3.277	3.164	3.178	3.11	3.140
Isoleucine	3.404	3.337	3.279	3.296	–	–	3.336	3.277	3.164	3.178	–	3.140
Lysine	3.467	3.400	3.345	3.360	–	–	3.401	3.339	3.416	3.430	–	3.213
Phenyl alanine	3.986	3.888	3.934	3.933	–	–	3.903	3.832	3.756	3.769	3.80	3.828
Valine	3.525	3.437	3.382	3.398	–	–	3.431	3.375	3.302	3.315	3.23	3.254
Threonine	3.942	3.846	3.829	3.842	–	–	3.834	3.770	3.664	3.679	3.71	3.729
Tyrosine	4.177	4.069	4.132	4.129	–	–	4.092	4.008	3.950	3.964	–	4.037
Tryptophan	4.140	4.060	4.070	4.066	–	–	4.098	4.005	3.959	3.972	4.03	4.045
Alanine	3.856	3.772	3.745	3.757	–	–	3.763	3.700	3.711	3.725	3.62	3.642
Histidine	4.280	4.169	4.239	4.235	–	–	4.182	4.106	4.057	4.073	–	4.156
Arginine	3.783	3.684	3.673	3.683	–	–	3.680	3.621	3.505	3.537	–	3.555
Aspartic acid	4.570	4.464	4.520	4.525	–	–	4.481	4.383	4.348	4.363	4.43	4.476
Glutamic acid	4.269	4.189	4.220	4.226	–	–	4.186	4.113	4.050	4.065	4.11	4.148
Glycine	4.222	4.086	4.096	4.106	–	–	4.102	4.008	3.927	3.962	–	4.013
Serine	4.191	4.088	4.093	4.104	–	–	4.091	4.008	3.926	3.942	–	4.013
Amino acid	Energy (keV)											
	302.9						356					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	3.341	3.278	3.210	3.221	–	3.143	3.355	3.275	3.282	3.284	–	3.147
Isoleucine	3.341	3.278	3.127	3.139	–	3.143	3.355	3.275	3.232	3.236	–	3.147
Lysine	3.405	3.337	3.307	3.320	–	3.215	3.409	3.337	3.252	3.254	–	3.218
Phenyl alanine	3.902	3.829	3.770	3.782	–	3.828	3.914	3.830	3.785	3.789	–	3.828
Valine	3.427	3.372	3.251	3.263	–	3.256	3.440	3.371	3.281	3.284	–	3.260
Threonine	3.854	3.772	3.669	3.683	–	3.729	3.838	3.768	3.691	3.693	–	3.729
Tyrosine	4.089	4.004	3.956	3.969	–	4.036	4.087	4.003	3.992	3.994	–	4.034
Tryptophan	4.094	4.004	3.968	3.980	–	4.044	4.107	4.003	3.988	3.991	–	4.042
Alanine	3.763	3.699	3.680	3.691	–	3.643	3.781	3.695	3.661	3.663	–	3.643
Histidine	4.188	4.106	4.066	4.080	–	4.154	4.182	4.105	4.090	4.093	–	4.151
Arginine	3.687	3.620	3.586	3.598	–	3.556	3.693	3.620	3.534	3.537	–	3.558
Aspartic acid	4.487	4.382	4.355	4.371	–	4.473	4.461	4.380	4.385	4.388	–	4.468
Glutamic acid	4.185	4.109	4.056	4.071	–	4.146	4.217	4.109	4.080	4.084	–	4.143
Glycine	4.134	4.005	3.966	3.980	–	4.012	4.125	4.006	3.958	3.961	–	4.010
Serine	4.083	4.004	3.934	3.949	–	4.012	4.106	4.006	3.959	3.961	–	4.010
Amino acid	Energy (keV)											
	383.9						661.6					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	3.345	3.275	3.262	3.257	–	3.149	3.341	3.273	3.236	3.242	3.18	3.162
Isoleucine	3.345	3.275	3.288	3.285	–	3.149	3.341	3.273	3.172	3.189	–	3.162
Lysine	3.392	3.336	3.240	3.236	–	3.220	3.400	3.334	3.233	3.238	–	3.232
Phenyl alanine	3.916	3.829	3.791	3.786	–	3.827	3.915	3.827	3.814	3.819	3.86	3.825
Valine	3.432	3.370	3.250	3.245	–	3.261	3.442	3.369	3.324	3.331	3.30	3.272

Table 5 continued

Amino acid	Energy (keV)											
	383.9						661.6					
	A	B	C	D	E	F	A	B	C	D	E	F
Threonine	3.844	3.768	3.787	3.783	–	3.729	3.854	3.766	3.715	3.751	3.74	3.730
Tyrosine	4.093	4.002	3.982	3.975	–	4.033	4.091	4.001	4.008	4.014	–	4.026
Tryptophan	4.092	4.002	3.992	3.987	–	4.041	4.085	4.001	4.014	4.021	4.06	4.034
Alanine	3.747	3.696	3.592	3.588	–	3.644	3.769	3.693	3.668	3.674	3.66	3.646
Histidine	4.196	4.104	4.079	4.074	–	4.150	4.183	4.101	4.119	4.127	–	4.139
Arginine	3.687	3.617	3.535	3.530	–	3.558	3.689	3.616	3.554	3.561	–	3.563
Aspartic acid	4.460	4.379	4.381	4.377	–	4.465	4.465	4.376	4.410	4.415	4.46	4.446
Glutamic acid	4.203	4.108	4.082	4.077	–	4.142	4.210	4.106	4.104	4.111	4.14	4.132
Glycine	4.115	4.002	3.971	3.966	–	4.009	4.128	4.001	3.984	3.990	–	4.002
Serine	4.084	4.002	3.960	3.953	–	4.009	4.081	4.001	3.985	3.990	–	4.002
Amino acid	Energy (keV)											
	1173						1332.5					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	3.371	3.273	3.274	3.282	3.17	3.177	3.372	3.273	3.279	3.278	3.13	3.180
Isoleucine	3.371	3.273	3.244	3.251	–	3.177	3.372	3.273	3.274	3.273	–	3.180
Lysine	3.439	3.334	3.314	3.318	–	3.245	3.432	3.334	3.348	3.350	–	3.248
Phenyl alanine	3.939	3.827	3.906	3.915	3.83	3.824	3.933	3.826	3.944	3.947	3.84	3.823
Valine	3.471	3.369	3.352	3.359	3.27	3.284	3.463	3.369	3.366	3.366	3.24	3.287
Threonine	3.877	3.765	3.812	3.822	3.73	3.731	3.870	3.766	3.842	3.843	3.73	3.731
Tyrosine	4.130	4.001	4.063	4.074	–	4.018	4.110	4.001	4.099	4.101	–	4.017
Tryptophan	4.128	4.001	4.038	4.049	4.04	4.026	4.116	4.000	4.048	4.051	4.01	4.024
Alanine	3.802	3.693	3.741	3.750	3.63	3.649	3.796	3.693	3.721	3.722	3.63	3.650
Histidine	4.215	4.101	4.223	4.234	–	4.129	4.221	4.101	4.154	4.156	–	4.126
Arginine	3.718	3.616	3.644	3.652	–	3.568	3.715	3.616	3.679	3.679	–	3.569
Aspartic acid	4.509	4.376	4.492	4.502	4.45	4.426	4.519	4.376	4.461	4.463	4.45	4.422
Glutamic acid	4.219	4.106	4.211	4.224	4.14	4.121	4.228	4.106	4.199	4.199	4.12	4.119
Glycine	4.152	4.001	4.034	4.044	–	3.996	4.162	4.001	4.011	4.013	–	3.994
Serine	4.109	4.001	4.084	4.095	–	3.996	4.125	4.001	4.118	4.123	–	3.994

A: MCNP-4C, B: XCOM, C: experimental [21, 22], D: Gowda et al. method [23], E: matrix method, and F: semiempirical formula given by Manjunathaguru and Umesh [24]

The effective electronic cross-section (σ_e) values of amino acids were calculated using Eq. (8) and are listed in Table 4.

As shown in Table 4, the effective electronic cross-section values of amino acids decreased with the increase in photon energy. Additionally, they were approximately independent of amino acid type, density, and molecular weight.

3.3 Effective atomic number and electron density of amino acids

The MCNP-4C, XCOM, and experimental [21, 22] values of the effective atomic number (Z_{eff}) and effective electron density (N_{eff}) of amino acids are given in Tables 5 and 6.

Additionally, the calculated effective atomic numbers and electron densities of some amino acids based on the formulae described by Manjunathaguru and Umesh [24] and Gowda et al. [23] are given in Tables 5 and 6.

Manjunathaguru and Umesh [24] calculated the effective atomic numbers and electron densities of some amino

Table 6 Effective electron density ($N_{eff} \times 10^{24}$ electron/g) of amino acids

Amino acid	Energy (keV)											
	81						276					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	0.344	0.337	0.333	0.335	–	–	0.337	0.331	0.320	0.321	0.314	0.317
Isoleucine	0.344	0.337	0.331	0.333	–	–	0.337	0.331	0.320	0.321	–	0.317
Lysine	0.343	0.336	0.331	0.332	–	–	0.336	0.330	0.338	0.339	–	0.318
Phenyl alanine	0.334	0.326	0.330	0.330	–	–	0.327	0.321	0.315	0.316	0.319	0.321
Valine	0.344	0.336	0.330	0.332	–	–	0.335	0.330	0.323	0.324	0.316	0.318
Threonine	0.339	0.331	0.329	0.331	–	–	0.330	0.324	0.315	0.316	0.319	0.321
Tyrosine	0.333	0.325	0.330	0.329	–	–	0.326	0.320	0.315	0.316	–	0.322
Tryptophan	0.330	0.323	0.324	0.326	–	–	0.326	0.319	0.315	0.316	0.321	0.322
Alanine	0.339	0.331	0.329	0.330	–	–	0.331	0.325	0.326	0.327	0.318	0.320
Histidine	0.332	0.324	0.329	0.329	–	–	0.325	0.319	0.315	0.316	–	0.323
Arginine	0.340	0.331	0.330	0.331	–	–	0.331	0.325	0.315	0.316	–	0.320
Aspartic acid	0.331	0.323	0.327	0.328	–	–	0.324	0.317	0.315	0.316	0.321	0.324
Glutamic acid	0.332	0.326	0.328	0.329	–	–	0.326	0.320	0.315	0.316	0.320	0.323
Glycine	0.339	0.328	0.329	0.329	–	–	0.329	0.322	0.315	0.316	–	0.322
Serine	0.336	0.328	0.328	0.329	–	–	0.328	0.322	0.315	0.316	–	0.322

Amino acid	Energy (keV)											
	302.9						356					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	0.337	0.331	0.324	0.325	–	0.317	0.339	0.331	0.331	0.332	–	0.318
Isoleucine	0.337	0.331	0.316	0.317	–	0.317	0.339	0.331	0.326	0.327	–	0.318
Lysine	0.337	0.330	0.327	0.328	–	0.318	0.337	0.330	0.321	0.322	–	0.318
Phenyl alanine	0.327	0.321	0.316	0.317	–	0.321	0.328	0.321	0.317	0.318	–	0.321
Valine	0.335	0.329	0.318	0.319	–	0.318	0.336	0.329	0.320	0.321	–	0.318
Threonine	0.331	0.324	0.315	0.317	–	0.321	0.330	0.324	0.317	0.318	–	0.321
Tyrosine	0.326	0.319	0.316	0.317	–	0.322	0.326	0.319	0.318	0.319	–	0.322
Tryptophan	0.326	0.319	0.316	0.317	–	0.322	0.327	0.319	0.318	0.318	–	0.322
Alanine	0.331	0.325	0.323	0.324	–	0.320	0.332	0.325	0.322	0.322	–	0.320
Histidine	0.325	0.319	0.316	0.317	–	0.322	0.325	0.319	0.318	0.318	–	0.322
Arginine	0.331	0.325	0.322	0.323	–	0.320	0.332	0.325	0.318	0.318	–	0.320
Aspartic acid	0.325	0.317	0.315	0.316	–	0.324	0.323	0.317	0.317	0.318	–	0.323
Glutamic acid	0.325	0.320	0.315	0.317	–	0.322	0.328	0.320	0.317	0.318	–	0.322
Glycine	0.332	0.321	0.318	0.319	–	0.322	0.331	0.321	0.318	0.318	–	0.322
Serine	0.328	0.321	0.316	0.317	–	0.322	0.329	0.321	0.318	0.318	–	0.322

Amino acid	Energy (keV)											
	383.9						661.6					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	0.338	0.331	0.330	0.329	–	0.318	0.337	0.331	0.327	0.327	0.321	0.319
Isoleucine	0.338	0.331	0.332	0.332	–	0.318	0.337	0.331	0.320	0.321	–	0.319
Lysine	0.335	0.330	0.320	0.320	–	0.318	0.336	0.330	0.320	0.320	–	0.320
Phenyl alanine	0.328	0.321	0.318	0.317	–	0.321	0.328	0.321	0.320	0.320	0.324	0.321
Valine	0.335	0.329	0.317	0.317	–	0.319	0.336	0.329	0.325	0.326	0.322	0.320

Table 6 continued

Amino acid	Energy (keV)											
	383.9						661.6					
	A	B	C	D	E	F	A	B	C	D	E	F
Threonine	0.330	0.324	0.325	0.325	–	0.321	0.331	0.324	0.319	0.320	0.322	0.321
Tyrosine	0.327	0.319	0.318	0.317	–	0.322	0.326	0.319	0.320	0.320	–	0.321
Tryptophan	0.326	0.319	0.318	0.318	–	0.322	0.325	0.319	0.320	0.320	0.323	0.321
Alanine	0.329	0.325	0.316	0.315	–	0.320	0.331	0.325	0.322	0.323	0.322	0.320
Histidine	0.326	0.319	0.317	0.316	–	0.322	0.325	0.318	0.320	0.320	–	0.321
Arginine	0.331	0.325	0.318	0.317	–	0.320	0.332	0.325	0.319	0.320	–	0.320
Aspartic acid	0.323	0.317	0.317	0.317	–	0.323	0.323	0.317	0.319	0.320	0.323	0.322
Glutamic acid	0.327	0.320	0.317	0.317	–	0.322	0.327	0.319	0.319	0.320	0.322	0.321
Glycine	0.330	0.321	0.319	0.318	–	0.322	0.331	0.321	0.320	0.320	–	0.321
Serine	0.328	0.321	0.318	0.317	–	0.322	0.327	0.321	0.320	0.320	–	0.321
Amino acid	Energy (keV)											
	1173						1332.5					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	0.341	0.331	0.331	0.331	0.320	0.321	0.341	0.331	0.331	0.331	0.316	0.321
Isoleucine	0.341	0.331	0.328	0.328	–	0.321	0.341	0.331	0.331	0.331	–	0.321
Lysine	0.340	0.330	0.328	0.328	–	0.321	0.339	0.330	0.331	0.331	–	0.321
Phenyl alanine	0.330	0.321	0.328	0.328	0.321	0.321	0.330	0.321	0.331	0.331	0.322	0.321
Valine	0.339	0.329	0.327	0.328	0.320	0.321	0.338	0.329	0.329	0.329	0.317	0.321
Threonine	0.333	0.324	0.328	0.329	0.321	0.321	0.333	0.324	0.330	0.330	0.321	0.321
Tyrosine	0.329	0.319	0.324	0.325	–	0.321	0.328	0.319	0.327	0.327	–	0.320
Tryptophan	0.329	0.319	0.322	0.322	0.322	0.321	0.328	0.319	0.322	0.323	0.319	0.320
Alanine	0.334	0.325	0.329	0.330	0.319	0.321	0.334	0.325	0.327	0.327	0.319	0.321
Histidine	0.327	0.318	0.328	0.329	–	0.321	0.328	0.318	0.322	0.323	–	0.320
Arginine	0.334	0.325	0.328	0.328	–	0.321	0.334	0.325	0.331	0.331	–	0.321
Aspartic acid	0.326	0.317	0.325	0.326	0.322	0.320	0.327	0.317	0.323	0.323	0.322	0.320
Glutamic acid	0.328	0.319	0.327	0.329	0.322	0.321	0.329	0.319	0.327	0.327	0.320	0.320
Glycine	0.333	0.321	0.324	0.324	–	0.321	0.334	0.321	0.322	0.322	–	0.320
Serine	0.330	0.321	0.328	0.329	–	0.321	0.331	0.321	0.330	0.331	–	0.320

A: MCNP-4C, B: XCOM, C: experimental [21, 22], D: Gowda et al. method [23], E: matrix method, and F: semiempirical formula given by Manjunathaguru and Umesh [24]

acids in the energy range of 145–1330 keV using two different methods: the new matrix method and the semiempirical relation for Z_{eff}. Additionally, Gowda et al. [23] obtained the semiempirical formula for Z_{eff} using a piecewise interpolation method.

At any photon energy of interest, it can be seen that the Z_{eff} values agree to within ± 7% for all amino acid samples based on various methods. Table 5 suggests that the effective atomic number values of each amino acid containing H, C, N, and O atoms are almost constant in the studied region of energy. Aspartic acid and isoleucine have the greatest and lowest values of Z_{eff}, respectively. This is due to the higher ratio of oxygen element content (up to 50%) in aspartic acid and the greatest effective atomic cross section of this amino acid compared to those of other amino acids.

Furthermore, the results shown in Table 6 indicate that the effective electron density of studied amino acids varies in the range of 3.14×10^{23}–3.44×10^{23} electron/g. In sum, it is evident from Table 6 that N_{eff} values are approximately identical and independent of the amino acid type in the studied energy regions.

Table 7 The theoretical and experimental values of μ_m (cm^2 g^{-1}) for alanine

Energy (keV)	81	276	302.9	356	383.9	661.6	1173	1332.5
XAAMDI	0.175	0.119	0.115	0.108	0.105	0.084	0.064	0.060
MCNP-4C	0.179	0.121	0.117	0.110	0.106	0.085	0.065	0.061
Difference (%)	2.21	1.13	1.70	1.81	1.12	1.57	2.61	2.50
XCOM	0.175	0.119	0.115	0.108	0.105	0.083	0.063	0.059
Difference (%)	0.00	0.00	0.00	0.00	0.00	− 0.49	− 0.32	− 0.28
Nair et al. [21, 22]	0.174	0.119	0.114	0.107	0.102	0.083	0.064	0.060
Difference (%)	− 0.75	0.00	− 0.56	− 1.40	− 3.06	− 1.17	0.00	0.00
Pawar and Bichile [7]	–	–	–	0.107	–	0.084	0.065	0.059
Difference (%)	–	–	–	− 1.40	–	0.00	2.61	− 0.28

Table 8 Mass attenuation coefficients (× 10^{-2} cm^2 g^{-1}) of some amino acids

Amino acid	Energy (keV)											
	356						661.6					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	0.112	0.110	–	0.107	–	–	0.087	0.084	–	0.083	–	–
Phenyl alanine	0.109	0.105	–	–	0.109	–	0.084	0.082	–	–	0.085	–
Threonine	0.110	0.105	–	–	0.109	–	0.085	0.082	–	–	0.086	–
Tryptophan	0.109	0.105	–	–	0.106	–	0.083	0.082	–	–	0.082	–
Alanine	0.110	0.107	–	0.107	–	–	0.085	0.083	–	0.084	–	–
Arginine	0.110	0.105	–	0.108	–	0.105	0.085	0.082	–	0.083	–	0.091
Glutamic acid	0.109	0.105	–	–	–	0.108	0.084	0.082	–	–	–	0.099
Glycine	0.110	0.105	0.107	0.104	–	–	0.085	0.082	0.084	0.084	–	–
Amino acid	Energy (keV)											
	1173						1332.5					
	A	B	C	D	E	F	A	B	C	D	E	F
Leucine	0.067	0.065	–	0.065	–	–	0.062	0.061	–	0.061	–	–
Phenyl alanine	0.065	0.064	–	–	0.064	–	0.060	0.061	–	–	0.059	–
Threonine	0.065	0.064	–	–	0.065	–	0.061	0.060	–	–	0.060	–
Tryptophan	0.064	0.063	–	–	0.062	–	0.060	0.059	–	–	0.061	–
Alanine	0.065	0.064	–	0.065	–	–	0.061	0.060	–	0.059	–	–
Arginine	0.065	0.064	–	0.063	–	0.067	0.061	0.061	–	0.058	–	0.053
Glutamic acid	0.064	0.064	–	–	–	0.060	0.060	0.060	–	–	–	0.058
Glycine	0.065	0.063	0.060	0.062	–	–	0.061	0.059	0.057	0.059	–	–

A: MCNP-4C; B: Nair et al. [21, 22], C: Pawar and Mahajan [1], D: Pawar and Bichile [7], E: More et al. [19], and F: Lokhonde et al. [18] values

3.4 Comparison with the XAAMDI database and other experimental data

The obtained values of mass attenuation coefficients for the amino acid alanine were compared with the theoretical values obtained from the XAAMDI (the X-ray Attenuation and Absorption for Materials of Dosimetric Interest) database using NIST (the National Institute of Standards and Technology) databases provided on the physical reference data web page to verify and validate theoretical (MCNP-4C and XCOM) and experimental results. The physical density of alanine was about 1.424 g cm^{-3} in this database. The μ_m values of the alanine amino acid obtained by MCNP-4C code simulation, XCOM program calculation, experimental measurements [7, 21, 22], and XAAMDI database calculation are presented in Table 7 for photon energies here. Additionally, the differences

between theoretical and experimental results obtained from the XAAMDI database are given in Table 7.

As shown in Table 7, the MCNP-4C, XCOM, experimental, and XAAMDI data are in good agreement with each other. The differences were found to be less than ± 3.1% for all methods. The maximum difference was observed − 3.06% for the data reported by Nair et al. [21, 22] at 383.9-keV photon energy. The other experimental data [7] showed good agreement with XAAMDI data with differences of ≤ ± 2.7%. XCOM presented the most analogous values to the XAAMDI data, with nearly full accordance, because both of them were developed for radiological physics and dosimetry by NIST and are based on the same theoretical calculations.

In addition, five experimental measurements [1, 7, 18, 19, 21, 22] of mass attenuation coefficients for some amino acids along with MCNP-4C data are given in Table 8.

It can be seen from Table 8 that the experimental measurements are up to ± 17.86% compared to each other. Except for the values reported by Lokhonde et al. [18] for a 661.6-keV photon energy, the differences of experimental results among each other and with MCNP-4C code data were less than ± 8%. However, all the experimental measurements were in good agreement with MCNP-4C code data and the μ_m values showed dependency on the photon energy (the μ_m values decreased with an increase in photon energy).

It should be noted that some observed differences in results could be because of the MCNP-4C code and the model itself, including the physical and mathematical models; uncertainties in the nuclear/atomic data; improper modeling of source energy and geometry; differences in experimental conditions like nuclear electronic setup and related errors; different physical conditions of the environment (pressure, humidity, and temperature); and different related errors in the measurement of physical quantities, like dimensions, densities, elemental composition of materials, and intensity of sources.

4 Conclusion

The μ_m, σ_a, σ_e, Z_{eff}, and N_{eff} values for fifteen essential amino acids in the energy range of 81–1332.5 keV were simulated and calculated using the MCNP-4C code and the XCOM program and were compared to available experimental and theoretical data. This study revealed that MCNP-4C simulation and XCOM calculations provide reliable photon interaction parameters for various amino acids within ± 7% RD values compared to the previous experimental data. The data calculated using the XCOM program showed better agreement with experimental data compared to MCNP-4C simulated results. It was found that the μ_m, σ_a, and σ_e values decreased with the increase in photon energy, while the Z_{eff} and N_{eff} values were almost constant in the studied region of energy for each amino acid. The data presented in this study would probably be beneficial in radiation dosimetry, health physics, and other radiation applications in the energy regions of interest.

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