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Calculation of effective atomic number and electron density of essential biomolecules for electron, proton, alpha particle and multi-energetic photon interactions

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HIGHLIGHTS

- We studied fatty acids, amino acids, carbohydrates and nucleotides.
- Calculations are done for charged particle interaction and multi-energetic photons.
- A non-monotonic variation occurs for protons and alphas at relatively low energies.
- A dramatic increase in Z_{eff} and N_e occurs for electrons at high-energy region.

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ABSTRACT

Effective atomic numbers (Z_{eff}) and electron densities (N_e) of some essential biomolecules have been calculated for total electron interaction, total proton interaction and total alpha particle interaction using an interpolation method in the energy region 10 keV^{-1} GeV. Also, the spectrum weighted Z_{eff} for multi-energetic photons has been calculated using Auto-Z_{eff} program. Biomolecules consist of fatty acids, amino acids, carbohydrates and basic nucleotides of DNA and RNA. Variations of Z_{eff} and N_e with kinetic energy of ionizing charged particles and effective photon energies of heterogeneous sources have been studied for the given materials. Significant variations in Z_{eff} and N_e have been observed through the entire energy region for electron, proton and alpha particle interactions. Non-uniform variation has been observed for protons and alpha particles in low and intermediate energy regions, respectively. The maximum values of Z_{eff} have found to be in higher energies for total electron interaction whereas maximum values have found to be in relatively low energies for total proton and total alpha particle interactions. When it comes to the multi-energetic photon sources, it has to be noted that the highest Z_{eff} values were found at low energy region where photoelectric absorption is the pre-dominant interaction process. The lowest values of Z_{eff} have been shown in biomolecules such as stearic acid, leucine, mannitol and thymine, which have highest H content in their groups. Variation in N_e seems to be more or less the same with the variation in Z_{eff} for the given materials as expected.

1. Introduction

High energy X-rays, gamma rays and particle radiation such as electrons, protons or heavy ions are of use in many applications viz. radioisotope monitoring, cross-section studies of absorption, scattering and attenuation of electromagnetic radiation, testing of multi-component, heterogeneous and composite materials etc. Besides, different types of ionizing radiation are being considered as therapeutic as well as diagnostic tools in radiotherapy and medical imaging (Foote et al., 1996; Kanematsu et al., 2012; Kramer et al., 1980; Jakob et al., 2005; Naydenov et al., 2004).

Among the parameters representing radiation attenuation through the materials such as mass attenuation coefficients for photons and stopping powers for electrons, protons and heavy ions, the effective atomic number and electron density are key parameters characterizing radiation response of different types of materials. They both have physical meanings and have been used in shielding as well as dosimetric applications. For example, deviations of the physical parameters such as effective atomic number by 15–20% from their normal values can be used to

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Table 1
Effective atomic number and electron density ($\times 10^{23}$) of fatty acids for electrons, protons and alpha particles.

Total electron interaction	Lauric acid		Palmitic acid		Stearic acid		Oleic acid		Myristic acid	
Kinetic energy (MeV)	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e
1.00E−02	2.76	1.47	2.72	1.47	2.70	1.47	2.75	1.49	2.74	1.47
5.00E−02	2.81	1.49	2.76	1.49	2.74	1.49	2.79	1.51	2.78	1.49
1.00E−01	2.82	1.50	2.77	1.50	2.75	1.50	2.81	1.52	2.79	1.50
5.00E−01	2.86	1.52	2.81	1.52	2.79	1.52	2.85	1.54	2.83	1.52
1.00E+00	2.85	1.52	2.80	1.52	2.78	1.51	2.84	1.54	2.82	1.51
5.00E+00	2.83	1.50	2.77	1.50	2.74	1.49	2.81	1.52	2.79	1.50
1.00E+01	2.88	1.53	2.82	1.52	2.78	1.51	2.86	1.55	2.83	1.52
5.00E+01	3.21	1.71	3.14	1.70	3.09	1.69	3.19	1.72	3.16	1.70
1.00E+02	3.40	1.81	3.32	1.80	3.28	1.79	3.37	1.82	3.35	1.80
5.00E+02	3.67	1.95	3.59	1.94	3.56	1.94	3.63	1.96	3.62	1.95
Total proton interaction	Lauric acid		Palmitic acid		Stearic acid		Oleic acid		Myristic acid	
Kinetic energy (MeV)	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e
1.00E−02	3.14	1.67	3.12	1.69	3.11	1.69	3.14	1.70	3.13	1.68
5.00E−02	3.31	1.76	3.27	1.77	3.25	1.77	3.30	1.79	3.29	1.76
1.00E−01	3.75	1.99	3.66	1.98	3.63	1.98	3.73	2.02	3.70	1.99
5.00E−01	2.96	1.57	2.89	1.56	2.87	1.56	2.94	1.59	2.92	1.57
1.00E+00	2.96	1.57	2.89	1.56	2.87	1.56	2.94	1.59	2.92	1.57
5.00E+00	3.02	1.60	2.95	1.60	2.93	1.60	3.00	1.62	2.98	1.60
1.00E+01	3.04	1.62	2.97	1.61	2.95	1.61	3.02	1.63	3.00	1.61
5.00E+01	3.06	1.63	3.00	1.62	2.97	1.62	3.04	1.65	3.02	1.62
1.00E+02	3.06	1.63	3.00	1.62	2.98	1.62	3.04	1.65	3.03	1.63
5.00E+02	3.07	1.63	3.00	1.63	2.98	1.62	3.05	1.65	3.03	1.63
Total alpha particle interaction	Lauric acid		Palmitic acid		Stearic acid		Oleic acid		Myristic acid	
Kinetic energy (MeV)	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e
1.00E−02	3.34	1.78	3.32	1.80	3.31	1.80	3.36	1.82	3.33	1.79
5.00E−02	3.23	1.72	3.20	1.73	3.19	1.74	3.24	1.75	3.21	1.72
1.00E−01	3.18	1.69	3.15	1.71	3.14	1.71	3.19	1.73	3.16	1.70
5.00E−01	3.23	1.72	3.17	1.72	3.15	1.72	3.21	1.74	3.20	1.72
1.00E+00	3.33	1.77	3.24	1.76	3.21	1.75	3.30	1.78	3.28	1.76
5.00E+00	2.96	1.57	2.89	1.56	2.87	1.56	2.94	1.59	2.92	1.57
1.00E+01	2.99	1.59	2.93	1.58	2.90	1.58	2.97	1.61	2.95	1.59
5.00E+01	3.04	1.62	2.98	1.61	2.95	1.61	3.02	1.63	3.00	1.61
1.00E+02	3.05	1.62	2.99	1.62	2.96	1.61	3.03	1.64	3.02	1.62
5.00E+02	3.07	1.63	3.00	1.62	2.98	1.62	3.05	1.65	3.03	1.63

Table 2
Effective atomic number and electron density ($\times 10^{23}$) of aminoacids for electrons, protons and alpha particles.

Total electron interaction	Alanine		Glutamine		Histidine		Leucine		Phenylalanine		Valine	
Kinetic energy (MeV)	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e
1.00E−02	3.49	1.63	3.74	1.74	3.99	1.89	2.98	1.48	3.67	1.81	3.09	1.51
5.00E−02	3.56	1.66	3.79	1.76	4.03	1.90	3.07	1.53	3.73	1.84	3.18	1.56
1.00E−01	3.58	1.67	3.81	1.77	4.04	1.91	3.10	1.54	3.75	1.85	3.21	1.57
5.00E−01	3.65	1.71	3.88	1.80	4.11	1.94	3.17	1.58	3.81	1.88	3.29	1.61
1.00E+00	3.65	1.70	3.88	1.80	4.11	1.94	3.16	1.57	3.81	1.88	3.28	1.61
5.00E+00	3.66	1.71	3.89	1.81	4.12	1.95	3.17	1.58	3.82	1.88	3.29	1.61
1.00E+01	3.74	1.75	3.96	1.84	4.19	1.98	3.26	1.62	3.89	1.92	3.38	1.65
5.00E+01	4.08	1.90	4.29	2.00	4.48	2.12	3.61	1.80	4.18	2.06	3.72	1.82
1.00E+02	4.25	1.98	4.45	2.07	4.61	2.18	3.78	1.88	4.32	2.13	3.89	1.90
5.00E+02	4.50	2.10	4.67	2.17	4.80	2.27	4.02	2.00	4.52	2.23	4.14	2.03
Total proton interaction	Alanine		Glutamine		Histidine		Leucine		Phenylalanine		Valine	
Kinetic energy (MeV)	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e	Z_{eff}	N_e
1.00E−02	3.44	1.61	3.54	1.65	3.67	1.74	3.28	1.63	3.53	1.74	3.32	1.63
5.00E−02	3.89	1.81	4.07	1.89	4.39	2.07	3.59	1.78	3.96	1.95	3.66	1.79
1.00E−01	4.49	2.10	4.66	2.17	4.86	2.30	4.14	2.06	4.58	2.26	4.22	2.07
5.00E−01	3.69	1.72	3.88	1.80	4.09	1.93	3.30	1.64	3.82	1.88	3.39	1.66
1.00E+00	3.64	1.70	3.81	1.77	3.98	1.88	3.27	1.63	3.75	1.85	3.36	1.64
5.00E+00	3.67	1.71	3.83	1.78	3.99	1.89	3.32	1.65	3.78	1.86	3.40	1.66