Radiation Physics and Chemistry 127 (2016) 48–55

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Studies on effective atomic numbers and electron densities of nucleobases in DNA

Ashok Kumar

College of Engineering and Management, Punjabi University Neighbourhood Campus, Rampura-Phul, Punjab, India

HIGHLIGHTS

- Effective atomic numbers and electron densities are calculated for nucleobases in DNA.
- Their variation has been studied with incident photon energy.
- Chemical composition of the nucleobases also influences the results.

ARTICLE INFO

Article history:
Received 29 August 2015
Received in revised form
8 June 2016
Accepted 10 June 2016
Available online 11 June 2016

Keywords:
Mass attenuation coefficients
Effective atomic number
Electron density
Nucleobases

ABSTRACT

Various parameters of dosimetric importance such as effective atomic numbers (Z_{eff}) and electron densities (N_{el}) of nucleobases in DNA have been calculated for the total and partial photon interaction processes in the wide energy range of 1 keV–100 GeV. The variations of Z_{eff} and N_{el} with energy are shown graphically for all partial and total interaction processes and are found to be similar. Up to 10 keV, Z_{eff} and N_{el} show a sharp increase for cytosine-guanine and thymine-adenine whereas for all the other nucleobases, it is almost constant. Then there is sharp decrease in Z_{eff} and N_{el} with energy up to 100 keV for all the nucleobases. From 100 keV to 6 MeV, Z_{eff} and N_{el} are almost independent of energy. From 6 MeV to 100 MeV, there is regular increase in Z_{eff} and N_{el} with photon energy. Above 400 MeV, Z_{eff} and N_{el} remain almost constant. The obtained results are due to the dominance of photoelectric absorption, Compton scattering and pair production in different energy regions as respectively stated above and their dependences on the chemical compositions of the interacting media.

1. Introduction

Accurate values of various parameters of dosimetric importance such as photon mass attenuation coefficients (μ_m), effective atomic numbers (Z_{eff}) and electron densities (N_{el}) are required to provide essential data in diverse fields such as nuclear diagnostics (computerized tomography), radiation protection, nuclear medicine, radiation dosimetry, gamma ray fluorescence studies, radiation biophysics etc. The μ_m is widely used in the calculation of photon penetration and energy deposition in dosimetric materials. It is a measure of probability of interaction that occurs between incident photons and matter of unit mass per unit area.

Hine (1952) has pointed out for photon interactions in composite materials that, a single number cannot represent the atomic number uniquely across the entire energy region, as in the case of pure elements. This number for composite materials is called "effective atomic number" and it varies with energy. The energy absorption in a given medium can be calculated if constants as Z_{eff} and N_{el} are known. This is useful in medical radiation dosimetry for the calculation of dose in radiation therapy and medical imaging. Therefore, the study of effective atomic numbers and electron density of biological samples is very useful for several technological applications.

Following the suggestions of Hine (1952), many attempts have been made to determine effective atomic number (Z_{eff}) for partial and total interactions in composite materials (El-Kateb and Abdul Hamid, 1991; Parthasaradhi, 1968; Perumallu et al., 1985; Lingam et al., 1984; Singh et al., 1996; El-Kateb et al., 2000; Nayak et al., 2001; Orhan and Salih, 2004; Orhan et al., 2005; Cevik et al., 2005, 2006; Baltas et al., 2007). Some empirically deduced formulae have also been reported (Shaltzer, 1979) but their validity is limited to the experimental conditions. Mudahar et al. (1991) has calculated Z_{eff} for different alloys. Ozyol (1994) evaluated the Z_{eff} for different biological materials and Singh et al. (2002) has measured Z_{eff} for different glasses. Gagandeep et al. (2000), Kaur et al. (2000) and Gowda et al. (2004) measured effective atomic

E-mail address: ajindal99@yahoo.co.in

http://dx.doi.org/10.1016/j.radphyschem.2016.06.006
0969-806X/

numbers and electron densities for some carbohydrates, alkali metal chloride-I and thermo-luminescent dosimetric compounds respectively in the medium energy range. Kurudirek (2011) estimated the effective atomic numbers of some solutions for photon energy absorption in the energy region 0.2 eV–1.5 MeV by an alternative method. The effective atomic number (Z_{eff}) of some rare earth compounds have been determined by Manjunatha and Umesh (2015) from the measured external bremsstrahlung (EB) intensity due to the incident beta particles emitted by the ^{90}Sr-^{90}Y source. El-Kateb and Abdul Hamid (1991) evaluated electron densities for several different substances containing C, H and O in the energy range from 54 keV. Hiremath and Chikkur (1993) and Manjunathaguru and Umesh (2006) have reported effective atomic numbers for some chemical compounds containing H, C, O and H, C, N, O atoms, respectively. Such studies in tissues and equivalent materials appear to be limited (Rao et al., 1985; Bhandal and Singh, 1993; Kumar and Reddy, 1997; Shivaramu et al., 1999; Shivaramu and Ramprasath, 2000; Shivaramu et al., 2001; Shivaramu, 2002; Salehi et al., 2015; Kurudirek, 2014). Taylor et al. (2012) proposed the Auto-Z_{eff} software for calculation of effective atomic numbers. Elmahroug et al. (2015) calculated the total mass attenuation coefficient, effective atomic number and the effective electron density for eight shielding materials in the energy range from 1 keV to 100 GeV. Un and Caner (2014) developed a Direct-Z_{eff} software for computation of the mass attenuation coefficient, the effective atomic number and the effective electron number per unit mass in the energy range 1 keV–100 GeV and compared its accuracy with calculated data and the experimental values for the various materials. Limkitjaroenporn et al. (2013) calculated the effective atomic number and electron density for the Inconel 738 superalloy from the measured values of the mass attenuation coefficient at different gamma ray energies by using the Compton scattering technique. Sharma et al. (2012) computed the effective atomic numbers from 1 keV to 100 GeV for different chemical compositions of calcium–strontium-borate glasses by two different methods: (a) the atomic to electron cross-section ratio and (b) logarithmic interpolation of molecular cross-section values. Sidhu et al. (2012) measured the total mass attenuation coefficient, total photon interaction cross-section, effective atomic numbers (Z_{eff}) and electron densities of low Z compounds of dosimetric importance at 59.54 keV photon energy emitted by 100mCi ^{241}Am point source employing narrow beam transmission geometry. Kore and Pravina (2014) measured the mass attenuation coefficients, the effective atomic numbers (Z_{eff}), and effective electron densities (N_{eff}) of some amino acids at 122, 356, 511, 662, 1170, 1275 and 1330 keV photon energies using a well-collimated narrow beam with good geometry set-up. Chantler (1995, 2000) studied the atomic form factors, photoelectric absorption, scattering cross-section and mass attenuation coefficients in the vicinity of absorption edges for the various element in the different energy regions. Other calculations of atomic form factors for measurement of attenuation coefficients are discussed elsewhere (Tran et al., 2003a, 2003b, 2005). Tran et al. (2005) used the x-ray-extended range technique to measure the x-ray mass attenuation coefficients of silver in the 15–50 keV energy range with a level of uncertainty between 0.27% and 0.4% away from the K-edge. A typical example of the method based on synchrotron radiation is the work of Chantler et al. (2001) for the measurement of the X-ray mass attenuation coefficient of copper using 8.85–20 keV synchrotron radiation.

Nucleobases are nitrogen-containing biological compounds found linked to a sugar within nucleosides—the basic building blocks of deoxyribonucleic acid (DNA). DNA molecules are considered to be a particularly sensitive target in biological systems, since primary and secondary radiation induces excitation or splitting of inorganic and organic molecules. When DNA molecules are damaged by radiation, thymine-adenine or cytosine-guanine base pairs in DNA may be changed. As an example, thymine–thymine base pairs may occur and molecular structures may be rendered unviable or may remain viable. The frequent and vital applications of radiation and its sources in medical and biological field advocates detailed knowledge of photon mass attenuation coefficients, effective atomic numbers and effective electron densities of selected nucleobases.

In the present work, the mass attenuation coefficients, effective atomic numbers and electron densities have been calculated for six nucleobases [adenine ($C_5H_5N_5$), guanine ($C_5H_5N_5O$), cytosine ($C_4H_5N_3O$), thymine ($C_5H_6N_2O_2$), cytosine-guanine ($C_{20}H_{27}N_7O_{13}P_2$) and thymine-adenine ($C_{19}H_{26}N_8O_{13}P_2$)] for all photon interactions [coherent, incoherent, photoelectric, pair production in nuclear as well as in the field of electron and total photon interaction (with coherent)] in the energy range 1 keV–100 GeV.

2. Theory

2.1. Mass attenuation coefficients

When a narrow beam of incident intensity I_0 passes through a homogeneous absorber of thickness x (cm), then according to Beer–Lambert's Law, the emerging photon intensity I is given by the following expression:

$$I = I_0 e^{-\frac{\mu}{\rho}\rho x} \tag{1}$$

where μ (cm^{-1}) is the linear attenuation coefficient for a material of mass density ρ(g/cm^3) and atomic number Z. The mass attenuation coefficient has the advantage of being independent from the material density. If the absorber is a chemical compound or a mixture, its mass attenuation coefficient μ/ρ can be approximately evaluated from the coefficients μ_i and ρ_i for the constituent elements according to the weighted averages

$$\mu/\rho = \sum_i w_i(\mu_i/\rho_i) \tag{2}$$

where w_i is the proportion by weight of the ith constituent.

2.2. Effective atomic number

The total molecular cross-section $\sigma_{t,m}$ can be calculated from the knowledge of mass attenuation coefficient by using the following relation:

$$\sigma_{t,m} = \left(\frac{\mu}{\rho}\right)\frac{M}{N_A} \tag{3}$$

where $M = \sum_i n_i A_i$ is the molar mass (molecular weight), N_A is Avogadro's constant, n_i and A_i are the number of formula atoms and the atomic weight of element i.

The average atomic cross-section $\sigma_{t,a}$ can be obtained by dividing the molecular cross-section by the total number of formula atoms as follows:

$$\sigma_{t,a} = \sigma_{t,m}\frac{1}{\sum_i n_i} \tag{4}$$

Similarly, the average electronic cross-section $\sigma_{t,el}$ is given by

$$\sigma_{t,el} = \frac{1}{N_A}\sum_i \frac{f_i A_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i \tag{5}$$

where $f_i = n_i/\sum_j n_j$ is the fractional abundance of element i with