Determination of Effective Atomic Number of Some Bimolecules for Electron Interaction.

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Abstract: *The effective atomic number of biomolecules such as carbohydrates and carboxylic acids for electron interaction at the energy of 942 keV have been determined by measuring their mass stopping power, using a Si(Li) detector coupled to 8K multichannel analyzer. The mass stopping power are determined by measuring the energies of incident electrons and transmitted electrons in the biomolecules. From the measured mass stopping power, the effective atomic numbers of the biomolecules have been determined and compared with theoretical values for electron interaction and photon interaction.*

Keywords: *Internal Conversion (IC), Mass Stopping Power (MSP), Effective Atomic Number (Z_{eff})*

I. Introduction

Effective atomic number (Z_{eff}) is widely used in radiation studies, particularly for characterizing the interaction processes in alloys, biological tissues and substitute materials. Hine[1] has pointed out that the atomic number of a composite material varies with the type of radiation and energy of the radiation with which it interacts. Effective atomic number can be defined as a weighted arithmetic mean of the atomic number of the constituent atoms. This weighing factor accounts for the type of radiation, material and interaction cross section. Several authors have determined the Z_{eff} for photon interaction ($Z_{eff,pi}$) at different energy ranges for various materials like semiconductors, polymers, inorganic compounds, alloys, dosimetric materials, thermo luminescence materials, biological samples and biological molecules as listed by Manohara et al.,[2]. Manjunathaguru et al., have derived semi empirical formula by matrix method to calculate $Z_{eff,pi}$ of biologically important compounds containing H,C,N,O in the energy range of 145 -1330 keV[3] and 6.4- 136 keV[4]. Manohara et al.,[5] have devised a comprehensive set of formulas for all types of materials and photon energies above 1 keV. Recently Singh and Badiger have compared various methods of calculating Z_{eff} of human organ tissue substitutes [6].

Unlike $Z_{eff,pi}$, the studies on Z_{eff} for electron interactions, $Z_{eff,ei}$, are very few. White[7] was the first to analyze the photon interaction and electron interaction in the matter and showed that Z_{eff} differs for photon and electron interactions. Parthasarathy et al.,[8] have calculated Z_{eff} of biological materials for photon, electron and He ions. Recently Kurudirek et al.,[9] have calculated Z_{eff} of many essential biomolecules for the photon, electron, proton and alpha particle interactions; the calculations are carried out for a variety of therapeutically significant energy ranges. Taylor et al., have calculated the Z_{eff} for radiative, collisional and total electron interaction processes in gel dosimetric materials [10] and in TLD-100 and TLD-100H dosimetric materials [11] over a wide range of energy.

All these authors obtained the Mass Stopping Power (MSP) values either from ICRU report-37 [12] or from ESTAR [13] and then established the relation between MSP and Z of the elements; the Bragg additivity law is used to compute the MSP of the sample. The $Z_{eff,ei}$ of the sample is taken as the Z corresponding to the MSP of the sample in the Z vs MSP plot of the elements. It is well known that the Bragg additivity law does not account for environmental effect and hence experimentally determined the MSP values will undoubtedly give information about environmental effect. In the present work, we have measured the MSP using Si(Li) detector spectrometer and determined the $Z_{eff,ei}$ of some biological samples using empirical formula.

II. Theoretical Background

Theoretical values of $Z_{eff,ei}$ are calculated using standard formula as given below:

$$Z_{eff,ei} = \frac{\sum_i Fi\ Ai(MSP)i}{\sum_i Fi\ Ai(MSP)i/Zi} \qquad (1)$$

where (MSP)i, Ai &Fi are the MSP, mass number & molar fraction of the element i in the mixture or compound. Theoretical values of $Z_{eff,pi}$ are calculated using Auto-Zeff software [14]. This is user-friendly software written in visual basic to compute the average atomic numbers and spectral-weighted mean atomic numbers. It determines $Z_{eff,pi}$ by establishing the smooth correlation between the interaction cross-section and the atomic number. It uses a matrix of mass attenuation coefficients formed as a function of atomic number and photon energies ranging from 10 keV to 1 GeV. The cross-sections of a compound or mixture are calculated by linear additivity and their $Z_{eff,pi}$ by the interpolation of Z values between adjacent cross-section data.

III. Experimental Procedure

The experimental arrangement to measure the MSP and the effective atomic number for electron is shown in Figure 1. It consists of radioactive Bi[207] internal conversion source, collimators and a Si(Li) detector, an ORTEC make preamplifier, an ORTEC make delay line amplifier and an 8K multichannel analyzer.

Bi[207] IC source emits 481.69, 555.39, 975.69 & 1049.39 keV internal conversion electrons and is supplied by New England Nuclear. The source is electroplated on a platinum foil and encapsulated in stainless steel of 1.52 cm outer diameter. It is covered with 18.8 mg/cm^2 thick beryllium window to prevent the source spilling and contamination. After correcting for the attenuation of these electrons in beryllium window and in air column between the source and detector, their effective energies are 443.98, 518.84, 941.74 and 1015.56 keV.

Two collimators C1 and C2 have been used to achieve good geometry in the present experiment. The collimator C1 is placed near the source and C2 near the detector. The internal conversion electrons are detected with the selection-grade NE Si(Li) detector which has 0.2cm depletion thickness and 15cm^2 active area. The output of the detector is fed to a charge sensitive preamplifier which has charge sensitivity 15 mV/MeV. The output of pre-amplifier in connected to a delay line amplifier and then to 8K multichannel analyzer. The entire assembly is placed in a light tight box.
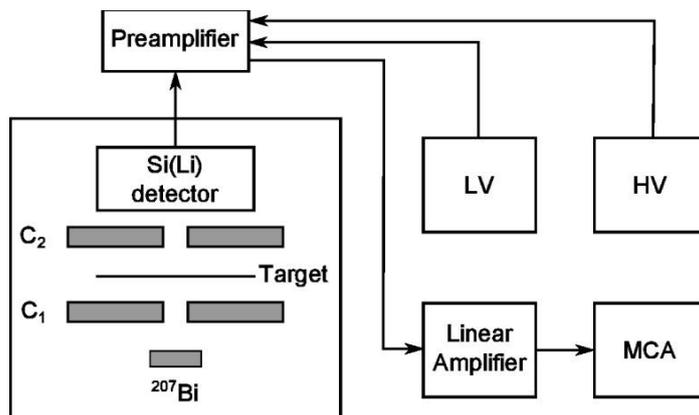

Fig.1. Experimental arrangement: C1, Source collimator; C2, Detector collimator; LV, Low voltage unit ; HV, High Voltage Unit; MCA, multichannel analyzer

A typical IC spectrum of Bi[207] obtained with Si(Li) detector spectrometer is shown in Figure 2. The four peaks at 443.98, 518.84, 941.74 and 1015.56 keV are fitted to Exponentially Modified Gaussian (EMG) to get the channel number corresponding to Most Probable Energy (MPE) of these peaks and fitting is Figure 2. The detector spectrometer is calibrated by plotting MPE against the corresponding channel numbers as shown in the Figure 3 and slope of the straight line gives the calibration constant which is (0.295±0.003) keV/channel.
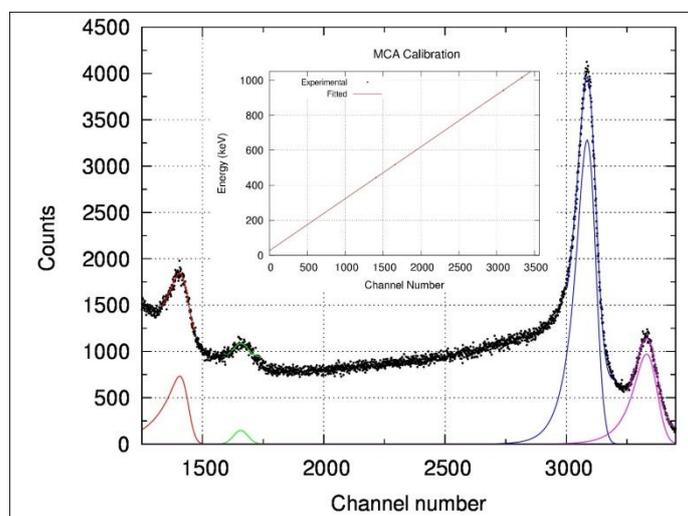

Fig.2. EMG fitted incident Bi[207] spectrum with MCA calibration graph.

In the present experiment, we have used 942 keV electrons as the incident electron for measuring MSP of the biomolecules. We have used two sample holders; one for carbohydrates (solid samples) and other for carboxylic acids (liquid samples). The energies of 942 keV electrons after correcting for the attenuation in the sample holders are 927.55 keV for carbohydrate sample holder and 911.23 keV for carboxylic acids sample holder. The carbohydrates samples and carboxylic acids sample are placed between collimators C1 and C2, and the transmitted electrons are measured with a Si(Li) detector spectrometer. The incident and transmitted spectra in carbohydrates samples and carboxylic acids sample are shown in Figure 4 and 5 respectively.
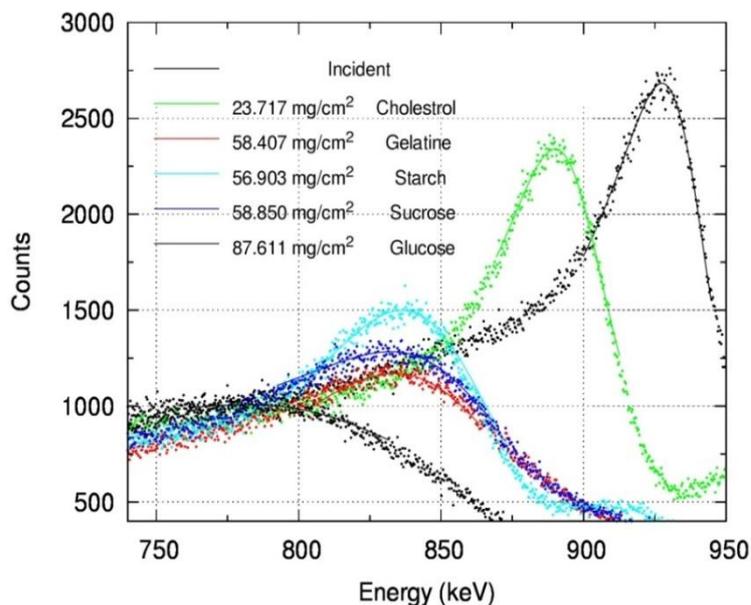
Fig.4. EMG fitted 928keV spectra incident on and transmitted by carbohydrates
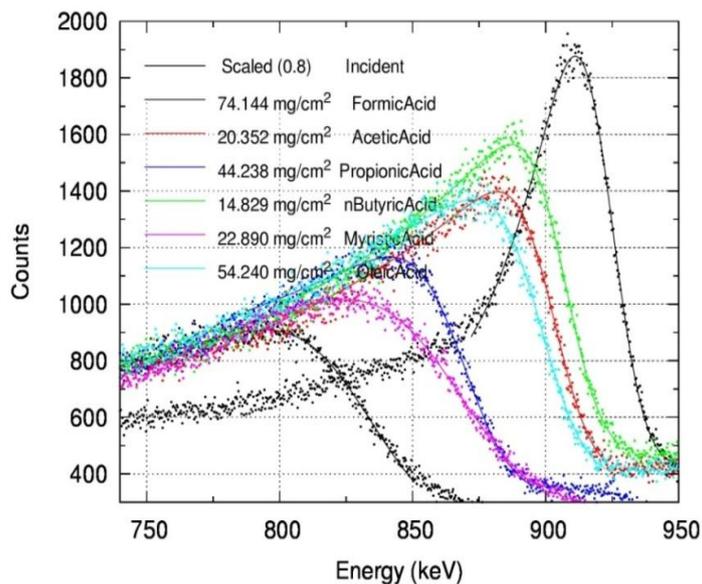
Fig.5. EMG fitted 911keV spectra incident on and transmitted by carboxylic acids.

IV.   Empirical Relation Between MSP and Atomic Number

In our earlier paper [15], we have established a semi empirical relation between the MSP and Z of elements for Z>10, and using that relation we have determined $Z_{eff,ei}$ of composite material by measuring their MSP values. But for Z< 10, it is difficult to measure their MSP values as most of the elements are in gaseous form at room temperature. In the present work, we have used ESTAR data[13] to obtain MSP values for hydrogen, carbon, nitrogen and oxygen at 911.22 keV and 927.54 keV electrons. In order to obtain a smooth curve, we have also included in figure, the MSP values of He and Be. The plot of MSP versus Z values yields an exponential type of curve as given in Figure 6.
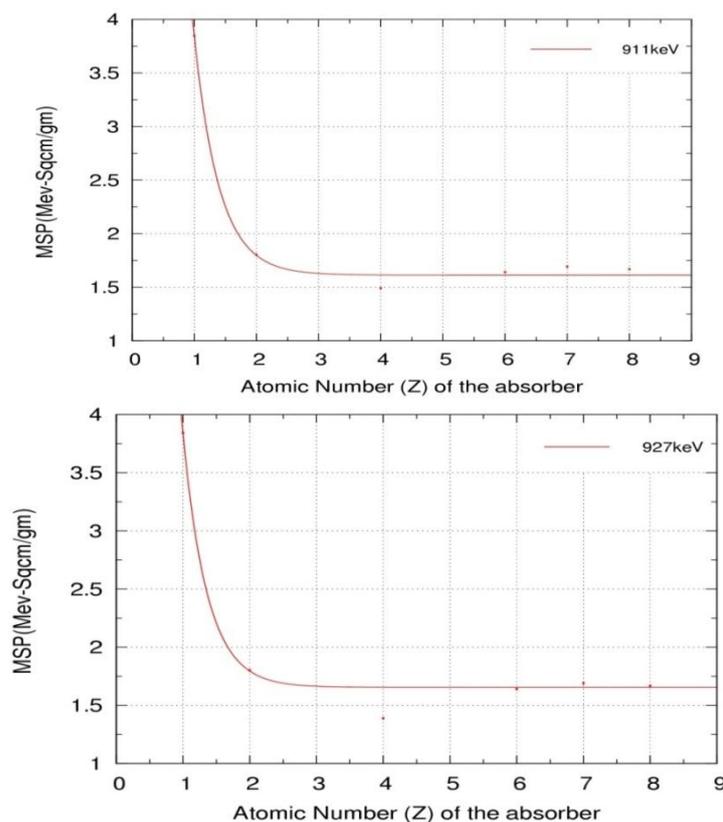
Fig.6. Exponential variation of MSP[13] with atomic number of H, He, C,N & O

The corresponding equation is given by equation 2 and fitting parameters are given in Table I.

$$MSP(MeV.cm^2/gm) = A_0 + A_1 e^{-BZ} \qquad (2)$$

From this exponential formula, $Z_{eff,ei}$ of carbohydrates and carboxylic acid can be determined by knowing the experimental MSP values and the constants A_0, A_1 and B.

Table I. Fitting parameters for the incident energies of 911 and 928 keV

E(keV)	A_0(MeV-cm^2/gm)	A_1(MeV-cm^2/gm)	B
911	1.6565	34.1107	2.7473
928	1.6549	34.1106	2.7488

V. Determination of Effective Atomic Number

The mass stopping power values of carbohydrates for 911 keV electrons are determined by measuring the incident energy and transmitted energy and by knowing the target thickness. These values are given in Table II. The $Z_{eff,ei}$ are determined using equation 2 by knowing experimental stopping power and the constants A_0, A_1 and B. In the same table, we have compared experimentally determined effective Z values with the values determined by direct method.

Table II. Experimental MSP (MeV-cm^2/gm) and $Z_{eff,ei}$ for carbohydrates.

Thickness mg/cm^2	Sample	MPE (keV)	Energy loss (keV)	MSP	$Z_{eff,ei}$ by Eq(1)	By direct method	
						$Z_{eff,ei}$	$Z_{eff,pi}$
7.360	Incident	927.547	...	...	...	...	...
23.009	Cholesterol	889.121	-38.426	1.670	2.809	2.735	2.920
56.637	Gelatin	833.804	-93.743	1.655	4.330	4.251	4.431
84.071	Glucose	788.345	-139.200	1.656	3.855	3.764	4.002
55.752	Starch	835.246	-92.301	1.656	3.962	3.862	4.097
55.522	Sucrose	832.308	-95.239	1.656	3.895	3.810	4.046

Similarly, the mass stopping power values of carboxylic acids for 928 keV electrons are determined by measuring the incident energy and transmitted energy and by knowing the target thickness. These values are given in Table III. The $Z_{eff,ei}$ are determined using equation 2 by knowing experimental stopping power and the constants A_0, A_1 and B. In the same table, we have compared experimentally determined effective Z values with the values determined using direct method.

Table III. Experimental MSP (MeV-cm^2/gm) and $Z_{eff,ei}$ for carboxylic acids

Thickness mg/cm^2	Sample	MPE (keV)	Energy loss (keV)	MSP	$Z_{eff,ei}$ by Eq(1)	By direct method	
						$Z_{eff,ei}$	$Z_{eff,pi}$
7.360	Incident	911.226	.....	.....	.....	.....	.....
69.666	Formic Acid	795.818	-115.408	1.657	4.704	4.582	4.940
19.407	Acetic Acid	879.061	-32.165	1.657	3.849	3.788	4.002
42.795	Propionic Acid	840.240	-70.986	1.659	3.507	3.434	3.638
14.431	n-Butyric Acid	887.266	-23.960	1.660	3.313	3.235	3.430
52.249	Myristic Acid	823.883	-87.342	1.672	2.810	2.741	2.910
21.895	Oleic Acid	874.639	-36.586	1.671	2.826	2.758	2.910

VI.   Results and Discussion

In the present experiment, we have used the Bi^{207} as the source of IC electrons which has the advantage that it emits wide range of mono energetic IC electrons all of them can be used for calibration of Si(Li) detector spectrometer. In the present experiment, we have studied mass stopping power of 942 keV electrons in biomolecules such as carbohydrates and carboxylic acids. From this mass stopping power, $Z_{eff,ei}$ for carbohydrates and carboxylic acids have been determined using our empirical relation as given in Eq.2. Thus obtained $Z_{eff,ei}$ values are compared with the $Z_{eff,ei}$ and $Z_{eff,pi}$ calculated by direct method. In the direct method, we have used standard formula to calculate $Z_{eff,ei}$ and Auto-Zeff software[14] to calculate $Z_{eff,pi}$. These values are given in Table II for carbohydrates and in Table III for carboxylic acid.

From the Table II for carbohydrates, we notice that our experimental $Z_{eff,ei}$ values closely agree with the theoretical values computed by direct method. Similarly from Table III for carboxylic acid, we have observed that our experimental $Z_{eff,ei}$ values are in close agreement with the values calculated using direct method. This establishes the correctness of our experimental setup, procedure and empirical formula as given in equation-2.

From the Table II and III, we also observe that both the experimentally determined as well as theoretically calculated values of $Z_{eff,ei}$ are slightly different from the $Z_{eff,pi}$ values. This corroborates that the effective atomic number for electron interactions and photon interactions are slightly different particularly at high energy of electron. Therefore, it is necessary to have more experimental data on Z_{eff} for electron interaction at high energy region.

Manohara et al.,[16] has established that the $Z_{eff,pi}$ for biological materials is energy-independent over a wide range of energies around 1MeV. In case of electron interaction too such constancy of MSP[13] and $Z_{eff,ei}$ could be observed around 1MeV. This made us to opt for the relatively high intense 942keV IC electrons of Bi^{207}.

VII.   Conclusion

From the above data we conclude that Z_{eff} depends on the type of radiation also and $Z_{eff,ei}$ of biomolecules can be determined accurately using Si(Li) detector spectrometer with good geometry arrangement. The close agreement of experimentally determined $Z_{eff,ei}$ values with that calculated using direct method shows the validity of our empirical relation between MSP and $Z_{eff,ei}$ of biomolecules. Whenever the value of MSP or $Z_{eff,}$ of biomolecules are not available in the literature, one can measure their MSP as outlined in this paper and obtain the $Z_{eff,ei}$ of biomolecules accurately using our empirical formula.

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