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Effective Atomic Number Dependence of Radiological Parameters of Some Organic Compounds at 122 KeV Gamma Rays

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Abstract Mass attenuation coefficient is a fundamental parameter of radiation interaction, from which the other radiological parameters like half Value Layer [HVL], tenth Value Layer [TVL], total atomic and electronic cross-sections, mass energy absorption coefficient, KERMA, CT number and effective atomic number are deduced. These parameters are extensively required in a number of fields such as diagnostic radiology, gamma ray spectroscopy, fluorescence analysis and reactor shielding. In the present work, mass attenuation coefficients are determined experimentally for some organic compounds at 122 keV incident photons using narrow-beam transmission geometry to establish a relation between effective atomic number (Z_{eff}) and other deduced parameters. The experimental data for all these parameters are compared with the values deduced from WinXcom software package and are found to agree within experimental estimated errors. This study gives some insight about the photon interaction in some organic compounds whose effective atomic numbers match with some human body fluids.

Keywords: Effective atomic number; mass-energy absorption coefficient; mass attenuation coefficient; HVL; CT number.

1. INTRODUCTION

The study of interactions of photons with material has an important role in the field of nuclear engineering, space technology, medicine and biology, agriculture and industry. The effective atomic number is a convenient parameter in atomic and nuclear radiation studies for interpreting the attenuation of

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X- or gamma-rays in complex medium such as biological tissue and particularly for the calculation of absorbed dose in radiation therapy. The gamma ray can interact with a target material by various processes depending upon the mode of interaction that cause scattering or complete absorption of gamma-ray photons. The scattering or complete absorption of gamma-rays and X-rays are closely related to the atomic number and electron density of an element. But in the case of composites/compounds, a single number can't represent the atomic number uniquely for the entire energy range as the partial interaction cross-sections have different Z dependence, as stated by Hine [1]. The effective atomic number is the ratio of total atomic cross-section to the total electronic cross-section for a mixture/compound and varies with incident photon energy that provides conclusive information of number of parameters. This radiological parameter has number of applications and is useful in dosimetric studies for calculation of radiation dose and shielding. Hubbell [2] evaluated the mass attenuation coefficient values of 40 elements and 45 mixtures/compounds in the energy region 1 keV-20 MeV. The calculated values of mass attenuation coefficient and mass energy absorption coefficient have been used widely as reference data in radiation shielding and dosimetry [3]. The WinXcom [4] software package had made possible to evaluate the effective atomic number with more accuracy. It also provides the information content for essential amino acids over wide range of incident photon energies above 1 keV-100 GeV [5]. The Pb-Sn alloys of various compositions, soldering material, Bakelite, Perspex, bronze, brass and scientific samples of rare earths materials were investigated to study the effective atomic number in a scattering geometry [6]. Several investigations [7-10] had determined the parameters like mass attenuation coefficient, effective atomic number, electron density, half value layer (HVL), tenth value layer (TVL), atomic and electronic cross-sections, and mass energy absorption coefficients.

The organic compounds used in the present investigations have many applications in medical, scientific, technological, industrial and biological fields. The mass attenuation coefficients (μ/ρ) are determined by measuring photo-peak areas under the Gaussian peak of the spectra of the ^{57}Co radioactive source with and without the target. All other radiological parameters for organic compounds like total atomic and electronic cross-sections (σ_t and σ_e), mass energy absorption coefficient (μ_{en}/ρ), molar extinction coefficient (ε), half and tenth value layer (HVL, TVL), KERMA (K_a) and CT number were determined from the experimental data of μ/ρ. The experimental results have been compared with the values obtained from WinXcom software package. The Z_{eff} dependence of all the parameters at incident photon energy of 122 keV established for all organic compounds.

2. THEORY

Mass attenuation coefficient is a fundamental parameter to be measured in the present experiment and other parameters are deduced from it. The linear and mass attenuation coefficients for the different target materials at various energies are determined in narrow-beam transmission geometry. This variation in intensity of transmitted beam is given by the Beer-Lambert relation as follows:

$$I = I_o e^{-(\mu/\rho)\rho x} \tag{1}$$

where I and I_o represent the transmitted (attenuated) and incident (un-attenuated) intensity under the photo-peak in the photon beam and ρ.x is the mass thickness of the material under study.

Practically, for large sized sample in the narrow-beam geometric experiment, the attenuation factor is still exponential factor but modified by two factors. The first factor is the geometry factor which depends essentially on the source geometry and involves the insertion of inverse square law for a point isotropic source. The second factor is the build-up factor that takes into account secondary photons produced in the absorber which reaches the detector.

The total mass attenuation coefficient for a chemical compound (mixture of elements) is additive and is given by mixture rule [11]. The mass attenuation coefficient (μ/ρ) for a chemical compound/mixture can be evaluated from the mass attenuation coefficients (μ/ρ_i) of the constituent elements according to their weighted averages as:

$$\left(\frac{\mu}{\rho}\right)_{\mathrm{Comp}} = \sum_i \omega_i \left(\frac{\mu}{\rho}\right)_i \tag{2}$$

where ω_i and $(\mu/\rho)_i$ are weight fraction and mass attenuation coefficient of i^{th} constituent element in the chosen compound respectively. For any compound, the weight fraction is given as

$$\omega_i = \frac{n_i.A_i}{\sum_i (n_j.A_j)} \tag{3}$$

Where A_i is the atomic weight and n_i is the formula unit of the i^{th} element constituent.

The half value layer (HVL) and tenth value layer (TVL) which are linear attenuation coefficient dependant, can be determined from following relations.

$$\mathrm{HVL} = \frac{\ln(2)}{\mu} \tag{4}$$

$$\mathrm{TVL} = \frac{\ln(10)}{\mu} \tag{5}$$

The total atomic cross-section (cm^2/atom) for the organic compounds can be determined from the measured values of $(\mu/\rho)_{\mathrm{Comp}}$ using the following relation:

$$\sigma_{\mathrm{t}} = \frac{\mathrm{A_i}}{\mathrm{N_A}}\left(\frac{\mu}{\rho}\right)_{\mathrm{Comp}} \tag{6}$$

Where N_A is the Avogadro's number in the units of atoms/mole. The total electronic cross-section (cm^2/electron) is given by:

$$\sigma_{\mathrm{e}} = \frac{1}{\mathrm{N_A}}\sum_{\mathrm{i}}\frac{\mathrm{f_i}\,.\,\mathrm{A_i}}{\mathrm{Z_i}}\left(\frac{\mu}{\rho}\right)_{\mathrm{Comp}} = \frac{\sigma_{\mathrm{t}}}{\mathrm{Z_{eff}}} \tag{7}$$

where f_i denotes the fraction of elements present in the compound such that $f_1+f_2+f_3+\ldots+f_i=1$, Z_i is the atomic number of the ith element in the compound andN_i is the total number of atoms of the constituting ith element.

The total atomic and total electronic cross sections are related to the effective atomic number of a compound using the following relation

$$\mathrm{Z_{eff}} = \frac{\sigma_{\mathrm{t}}}{\sigma_{\mathrm{e}}} \tag{8}$$

The mass energy absorption coefficients were calculated by using the following relation:

$$\frac{\mu_{\mathrm{en}}}{\rho} = \frac{\sigma_{\mathrm{m,en}}\,.\,\mathrm{N_A}}{\mathrm{N}} \tag{9}$$

Kerma (K_a) has been computed using the known mass energy absorption coefficient of the compound $(\mu_{en}/\rho)_{Comp}$ and mass energy absorption coefficient values of water $(\mu_{en}/\rho)_{Water}$ with the following expression:

$$K_a = \frac{(\mu_{en}/\rho)_{Comp}}{(\mu_{en}/\rho)_{water}} \tag{10}$$

For interpreting the CT scans, a parametric CT number (computed tomography number) is widely used and is a normalized X-ray absorption coefficient of a pixel in a computer tomogram, expressed in Hounsfield units (HU) and can be calculated as

$$CT = 1000\left(\frac{(\mu_l)_{comp}}{(\mu_l)_{water}} - 1\right) \tag{11}$$

where $(\mu_l)_{comp}$ and $(\mu_l)_{water}$ are the linear attenuation coefficient for the gamma-ray in a compound and water respectively. The values of CT number for air is taken as -1000 HU and for water 0 HU, providing two independent calibrations points at two energies. The energy-dependence of the linear attenuation coefficients values of the organic compounds taken in this work is different from that of water.

3. EXPERIMENTAL METHOD AND MEASUREMENTS

The schematic arrangement of the experimental set-up for 'narrow-beam transmission geometry' is shown in the Fig. 1. The samples were irradiated by a radioactive point source of ^{57}Co (122 keV of strength 167 kBq) placed in the source housing. For each sample, the incident intensity I_o and transmitted intensity I of the gamma-rays is detected using NaI (Tl) scintillation (crystal dimensions of 51 mm diameter and 51 mm thickness) spectrometer and MCA plug-in card that records incident and transmitted gamma photon flux. The radioactive source and scintillation detector are properly shielded with lead bricks having dimensions of 16 × 8 × 4 cm^3. The organic samples filled in a thin walled cubic container of dimensions of 5 × 5 × 5 cm^3 were placed between source and detector to record I and I_o. The sample thicknesses were selected in order to satisfy criterion $\mu t \ll 1$ for precise measurements of attenuation coefficients [12]. The collimators of diameter 0.8 cm and 0.6 cm were placed

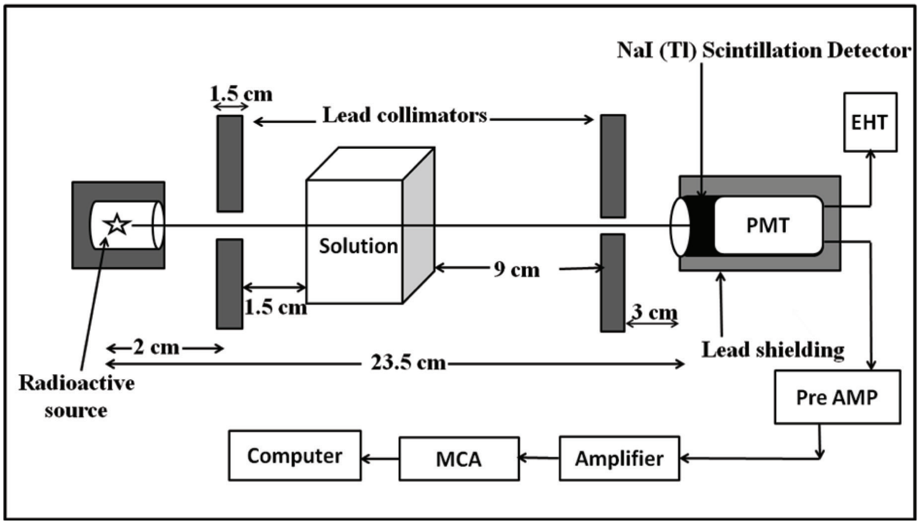

Figure 1: The schematic view of experimental set-up.

at a distance of 2 and 3 cm from source and detector to collimate the primary gamma beam and transmitted gamma flux, respectively. The properly shielded NaI (Tl) scintillation detector is placed at a distance of 23.5 cm from the source and is used to detect the signal from the organic compounds. The distances of the front face of target sample is placed at a 1.5 cm from source collimator and at 9 cm from detector collimator respectively. It has been checked experimentally that the background near the detector assembly comes out to the natural background level when the collimator opening of the radioactive source is closed. The measurements for all organic compounds were carried out using the following procedure;

Firstly, source spectra recorded with the empty container placed in the primary gamma-ray beam from ^{57}Co. Secondly, transmission spectra with the container filled with desired organic solutions for the same duration of time. Finally, by integrating the incident and transmitted spectra over the selected width of the photo-peak, incident intensity (I_o) and transmitted intensity (I) were obtained as shown in curve (a) and (b) of figure (2) respectively. The comparison of counting rate under the photo-peak without sample in the primary beam confirms that the attenuation resulting from the cubic container was found to be negligible. Each spectrum was recorded for sufficient time to accumulate adequate number of counts under the full energy peak to limit the uncertainty less than 1%. The probability of any shift in photo-peak of spectrum was checked from time to time to achieve accuracy. The half-angle of the cone of acceptance of the detector at the sample is taken as angular aperture of the geometry (θ) and calculated to be 1.07° which shows negligible amount of scattering contribution is involved in the mass attenuation coefficient measurement.

The experimental uncertainties in the present measurements are mainly due to counting statistics, multiple scattering effects, non-uniformity of the absorber, impurity content present in the sample, in the determination of mass thickness of the sample, evaluation of area under the photo-peak, possible errors resulting from the small angle scattering contribution and dead time of the counting detector. But, care has been taken while considering the contributions of the errors in the present investigations in order to minimize the errors propagation. Care has also been taken to maintain the homogeneity of the sample during the measurement.

4. RESULTS AND DISCUSSION

The organic compounds, their chemical formulae, density and molar mass used in the present work are listed in Table 1. The mass attenuation coefficient, half

Table 1: Data for organic compounds used in the present study at 122 keV.

Chemicals	**Chemical formula**	**Density (gm/cm²)**	**Molar Mass (gm/mole)**	$\mathbf{Z_{eff}}$	
				$\frac{\sigma_t}{\sigma_e}$	$\frac{\sum f_i \cdot Z_i}{\sum f_i}$
Isoamyl Alcohol	$C_5H_{12}O$	0.81	88.148	2.818	2.795
Butanone	C_4H_8O	0.805	72.11	3.086	3.105
Ethyl Benzene	C_8H_{10}	0.866	106.17	3.147	3.211
Cyclohexanone	$C_6H_{10}O$	0.948	98.15	3.189	3.228
Propylene Glycol	$C_3H_8O_2$	1.036	76.09	3.245	3.239
Acetone	C_3H_6O	0.791	58.08	3.256	3.273
Benzyl amine	C_7H_9N	0.981	107.153	3.426	3.394
Ethylene Glycol	$C_2H_6O_2$	1.11	62.068	3.443	3.437
Water	H_2O	0.997	18.015	3.444	3.445
Glycerin	$C_3H_8O_3$	1.261	92.094	3.57	3.602
Aniline	$C_6H_5NH_2$	1.022	93.126	3.585	3.603
Ethyl Formate	$C_3H_6O_2$	0.917	74.1	3.609	3.634
Glutaraldehyde	$C_5H_8O_2$	1.06	100.116	3.636	3.666
Acetophenone	C_8H_8O	1.03	120.15	3.733	3.799

Cinnamaldehyde	C_9H_8O	1.05	132.16	3.954	3.921
Benzaldehyde	C_7H_6O	1.04	106.121	3.977	4.019
Furfural	$C_5H_4O_2$	1.16	96.09	4.511	4.587
Nitrobenzene	$C_6H_5NO_2$	1.199	123.06	4.6	4.589

value layer, tenth value layer, molar extinction coefficient, total atomic cross-section, total electronic cross-section, mass energy absorption coefficient, kerma and CT number values for organic compounds have been determined and tabulated as function of Z_{eff} at 122 keV incident photon energy in Table 2 for narrow-beam transmission set-up (Fig. 1) along with the theoretical data. Z_{eff} values are determined from our experimental data by the ratio $\left(\sigma_t / \sigma_{te}\right)$ and theoretically using mixture rule and are found to be in agreement with each other. The values of Z_{eff} determined from the two different formulae are also included in the column 5 and 6 of Table 2. Fig. 2 shows a typical transmission spectrum for the case of ethylene glycol for 122 keV incident photons. Curve (a) is for the empty container and curve (b) is for the container filled with the ethylene glycol. In order to minimize the error caused due to fluctuations in photon intensity and sample thickness, data was taken in sequence and number of individual measurement on particular organic sample were performed. The

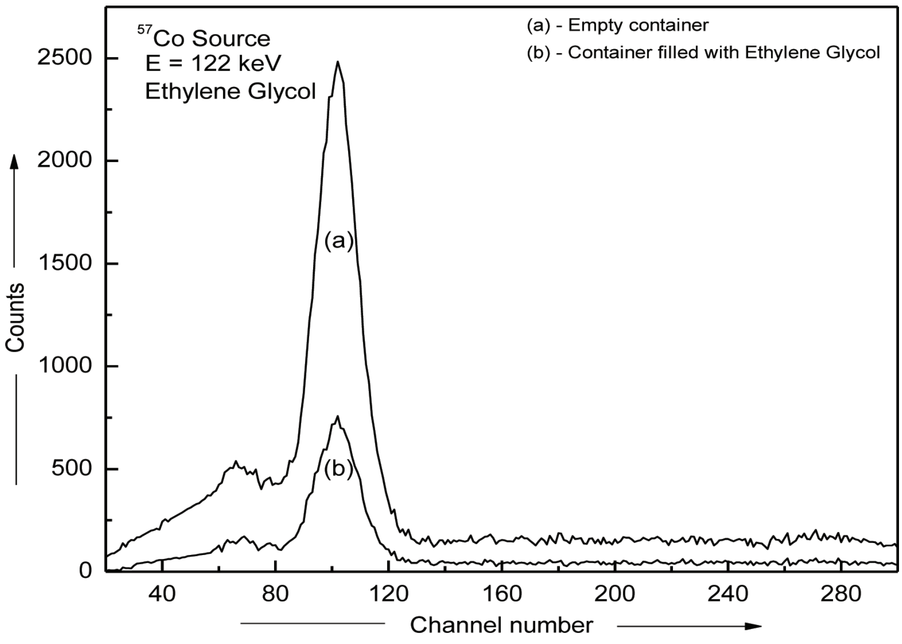

Figure 2: A typical Spectrum of ^{57}Co for Ethylene glycol.

Table 2: Radiological parameters as a function of effective atomic number (Z_{eff}) at 122 keV.

Zeff	Mass Attenuation Coefficient		HVL		TVL		Total atomic cross section		Total electronic cross section		Mass Energy Absorption coefficient		KERMA		CT number	
	Present Results	Theory	Present Results	Theory	Present Results	Theory	Present Results	Theory	Present Results	Theory	Present Results	Theory	Present Results	Theory	Present Results	Theory
2.818	0.164	0.162	5.2	5.282	17.263	17.536	1.337	0.931	0.464	0.481	0.057	0.059	1.207	1.223	−189.757	−184.724
3.086	0.159	0.159	5.409	5.414	17.959	17.975	1.465	1.009	0.471	0.476	0.051	0.051	1.07	1.08	−220.803	−204.792
3.147	0.152	0.156	5.257	5.13	17.452	17.03	1.49	1.065	0.483	0.462	0.049	0.047	1.002	1.016	−196.1	−160.679
3.189	0.157	0.158	4.639	4.626	15.4	15.359	1.511	1.057	0.473	0.475	0.049	0.049	1.03	1.038	−88.69	−69.41
3.245	0.156	0.159	4.286	4.208	14.231	13.969	1.517	1.09	0.481	0.469	0.049	0.048	1.019	1.025	21.239	23.413
3.256	0.16	0.158	5.453	5.544	18.105	18.406	1.549	1.045	0.464	0.484	0.048	0.05	1.022	1.032	−228.061	−223.494
3.426	0.155	0.155	4.551	4.556	15.109	15.127	1.624	1.126	0.471	0.476	0.045	0.045	1.07	0.951	−71.368	−55.275
3.443	0.158	0.158	3.939	3.951	13.079	13.117	1.633	1.112	0.471	0.48	0.045	0.046	0.962	0.967	73.066	89.644
3.444	0.165	0.161	4.202	4.318	13.949	14.335	1.649	1.13	0.46	0.494	0.046	0.049	1.001	0.998	0	0
3.57	0.159	0.156	3.452	3.523	11.462	11.697	1.739	1.202	0.463	0.486	0.042	0.044	0.904	0.913	193.712	222.23
3.585	0.154	0.154	4.404	4.406	14.62	14.627	1.701	1.207	0.472	0.476	0.042	0.043	1.038	0.902	−40.322	−22.439
3.609	0.153	0.155	4.934	4.877	16.382	16.191	1.713	1.198	0.478	0.471	0.04	0.042	0.883	0.892	−143.158	−116.94
3.636	0.155	0.155	4.199	4.218	13.942	14.003	1.725	1.213	0.47	0.479	0.042	0.043	0.891	0.9	6.643	20.803
3.733	0.15	0.153	4.474	4.397	14.855	14.599	1.765	1.259	0.48	0.468	0.041	0.04	0.841	0.85	−51.362	−20.886
3.954	0.156	0.152	4.23	4.342	14.045	14.416	1.902	1.279	0.46	0.489	0.037	0.04	0.809	0.818	−13.728	−8.398
3.977	0.150	0.151	4.438	4.414	14.734	14.655	1.889	1.331	0.475	0.472	0.037	0.037	0.782	0.793	−47.885	−24.303
4.511	0.148	0.15	4.034	3.983	13.391	13.223	2.148	1.539	0.48	0.472	0.033	0.032	0.683	0.689	47.814	81.069
4.6	0.150	0.149	3.85	3.878	12.783	12.875	2.19	1.517	0.47	0.479	0.032	0.032	0.758	0.685	97.707	109.96

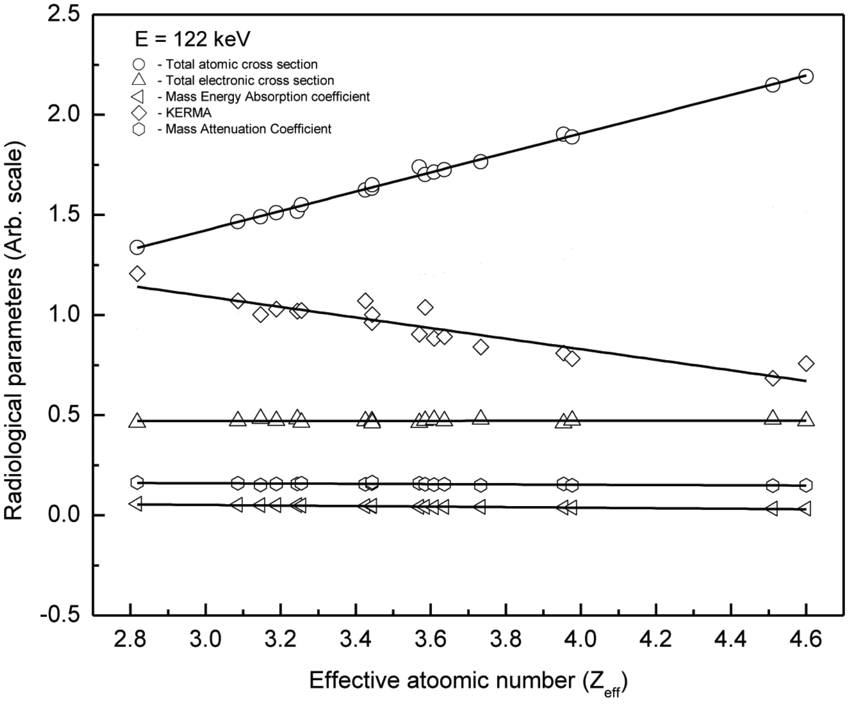

Figure 3: Variation of experimental values of radiological parameters for all organic compounds as a function of Z_{eff} values at 122 keV.

mass attenuation coefficients as a function of Z_{eff} are given column 2, 3 of Table 2. The peak areas have been evaluated from the spectra for each of the measurements. The estimated error in the experimental measurement was nearly 4%. The compounds selected for the measurements have Z_{eff} in the range 2.818-4.600 at 122 keV that simulates some of the fluids in human body. The mass attenuation coefficients slightly decrease with increase in Z_{eff} of compounds taken in the present study and are in agreement with the theoretical data evaluated with WinXcom within statistical uncertainty.

The experimental and theoretical values of HVL and TVL are determined using eqn. 4 and 5 respectively, and are given in column 4, 5 and 6, 7 of Table 2. There is decrease in these values with increase in Z_{eff} at 122 keV incident photons. As it is expected that with increase in Z_{eff}, HVL and TVL should decrease so this material can be used for radiation shielding purpose, but these measurements do not prove this aspect completely, but it proves the trend of the measurements for such a small range of Z_{eff}.

The values of total atomic and total electronic cross-sections are determined experimentally using eqns. 6 and 7 respectively at 122 keV. The experimental and theoretical results are given in column 8, 9 and 10, 11 of Table 2. The experimentally measured values of cross-sections agree well with the theoretical values computed by WinXcom. It is clear from the tables that the total atomic cross-section values increases with increasing effective atomic number for the organic compounds and total electronic cross-section values remain constant with Z_{eff}.

The mass energy absorption coefficients evaluated using eqn. (9) are given in Table 2 column 12, 13. The figure 3 shows the slight decrease of experimental values for the organic compounds at 122 keV with increase in Z_{eff} and are in agreement with the theoretical data.

The experimentally measured and theoretically calculated (using eqn. 10 and 11) values of kerma and CT number given in Table 2 (columns 14, 15 and 16, 17) for all the compounds at 122 keV incident energy. The kerma values linearly decreases with increase of effective atomic number, while the trend of CT number with respect to the Z_{eff} is slightly increasing with increase in the values of effective atomic number. There is a peak like structure near the Z_{eff} of water, which is due to slight variation of linear attenuation coefficient of water results in large values of CT number as it is clear from the expressions of eq. (11).

There are no measurements of all the radiological parameters of organic compounds used in the present study at 122 keV incident gamma photons to be compared with our experimental results.

5. CONCLUSIONS

In the composite materials, the gamma interaction through absorption is related to the Z_{eff} values and energy of the incident photons. Z_{eff} value is quite sensitive and useful parameter for composite materials of scientific, industrial, environmental, agricultural, geological, biological and medical interest. Z_{eff} is a dimensionless parameter which indicates many characteristics of materials. It provides estimation of chemical composition of the compound/mixture. Z_{eff} values are also utilized in radiation therapy to compute the absorbed dose. The measured values of mass attenuation coefficient (μ / ρ), mass energy absorption coefficients (μ_{en} / ρ) half value layer thickness, kerma relative to water, total atomic cross-sections (σ_t) and total electronic cross-section (σ_e) for all organic compounds containing H, C, N and O elements. Also, the trend of the variation of (σ_t) and (σ_e) with effective atomic number is identical with that of μ_{en} / ρ. Due to small scattering angle made at the aperture of the detector, the probability of scattering in these measurements was considered to be negligible. To our best of knowledge, there are no experimental investigations of $\mu/\rho, \sigma_{t}, \sigma_{te}, \mu_{en}/\rho$, HVL and K_a versus Z_{eff} in the literature for comparison with the present experimental results for the organic compounds used in the present work. It is further planned to perform measurements of μ/ρ with elements, compounds/mixtures, composite materials and alloys at other energies.

REFERENCES

[1] G. J. Hine, Phys. Rev., **85**, 725 (1952).

[2] J. H. Hubbell, Int. J. Appl. Radiat. Isot., **33**, 1269 (1982). https://doi.org/10.1016/0020-708X(82)90248-4

[3] J. H. Hubbell and S. M. Selzer, NISTIR, 5632 (1995).

[4] L. Gerward, N. Guilbert, K. B. Jensen and H. Levring, Radiat. Phys. Chem., **71**, 653 (2004).

[5] S. R. Manohara and S. M. Hanagodimath, Nucl. Instr. and Meth. B, **258**, 321 (2007). https://doi.org/10.1016/j.nimb.2007.02.101

[6] M. P. Singh, B. S. Sandhu and B. Singh, Phys. Scripta, **76**, 281 (2007). https://doi.org/10.1088/0031-8949/76/4/001

[7] I. Akkurt, S. Kilincarslan and C. Basyigit, Ann. Nucl. Eng., 31, 577 (2004). https://doi.org/10.1016/j.anucene.2003.07.002

[8] I. Han and L. Demir, J. X-Ray Sci. Techno., **18,** 39 (2010).

[9] M. Buyukyildiz, M. Kuurudirek, M. Ekici, O. Icelli and Y. Karabul, Prog. Nucl. Energ., **100,** 245 (2017). https://doi.org/10.1016/j.pnucene.2017.06.014

[10] S. R. Manohara, S. M. Hanagodimath and L. Gerward, J. Nucl. Mater., **393,** 465 (2009). https://doi.org/10.1016/j.jnucmat.2009.07.001

[11] D. F. Jackson and D. J. Hawkes, Phys. Rep., **70**, 169 (1981). https://doi.org/10.1016/0370-1573(81)90014-4

[12] D. C. Creagh, Nucl. Instrum. Methods A, **255**, 1 (1987). https://doi.org/10.1016/0168-9002(87)91064-3