Indian Journal of Pure & Applied Physics
Vol. 54, May 2016, pp. 333-338

Effective atomic numbers of dosimetric interest organic compounds

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Received 25 October 2013; revised 18 April 2014; accepted 13 January 2015

Effective atomic numbers of some dosimetric interest organic compounds, like glucose, ethanol, acetic acid, trichloroethylene, chloroform, benzene, acetone, phenol, chlorobenzene, naphthalene, adenine, alanine, anthracene, carbon tetrachloride, diethyl either and sucrose are calculated using Auto-Z_{eff}, direct, logarithmic interpolation, ratio, power law and single-value XmuDat methods. The calculated effective atomic numbers are compared with experiment data wherever possible and results show a good agreement. The Auto-Z_{eff}, direct, logarithmic interpolation and ratio methods are the most suitable for intermediate photon energy (50 keV < E < 20 MeV), where Compton scattering dominates. Mixture law is applicable in intermediate energy region for computation of theoretical effective atomic numbers. Kerma relative to air of the selected organic compounds are also calculated for photon energy 1 keV - 20 MeV. The kerma reaches unity beyond 200 keV and up to 10 MeV.

Keywords: Auto-Z_{eff}, Power law, Compton scattering, Dosimetric interest organic compound, Effective atomic number

1 Introduction

Application of radiation in nuclear engineering, nuclear physics, health physics, radiation physics, medical physics, radiation dosimetry, radiation protection, space research and radiobiology require knowledge of radiation interaction with the materials for shielding and dose measurement. Mass attenuation coefficients and effective atomic numbers are two essential parameters for composite or compound materials. It is to be noted that the effective atomic number is mainly important parameters used for initial assessment of dose, shielding efficiency and buildup factors. Studies on effective atomic numbers are available for different composites/mixtures such as building materials[1], gaseous mixtures[2], composite materials[3], thermo-luminescent dosimeters[4], dosimetric interest[5] and biological materials[6,7].

It is possible to evaluate the effective atomic number by various methods, such as ratio of atomic to electronic cross-section[8] (henceforth called ratio method), direct[9], Auto-Z_{eff}[10], logarithmic interpolation[11], power law[12] and XmuDat[13]. The average atomic number is calculated using arithmetic mean of atomic number using chemical formula $\langle Z \rangle = \frac{1}{n}\sum_i n_i Z_i$, where $n = \sum_i n_i$. The presence of different theoretical methods encouraged the authors to investigate the suitable method for calculation of effective atomic numbers. The non-validity of mixture rule has been reported near *k*-absorption edge[14]. In the present work, some dosimetric interest organic compounds as given in Table 1 are considered. The kinetic energy released per unit mass (Kerma) of the organic compound is also calculated for photon energy from 1 keV to 20 MeV. The theoretical results are compared with possible experimental data and a very good agreement is found.

2 Theoretical Background and Computation Work

2.1 Mass attenuation coefficients

Mass attenuation coefficient and cross-section data for elements in the photon energy range of 1 keV - 100 GeV are given by XCOM program[15], which has been transformed to user-friendly software WinXCom[16] on Windows operating system. The mass attenuation coefficients, μ/ρ of the organic compounds are calculated by mixture rule[17] ($(\mu/\rho)_{compound} = \sum_i^n w_i (\mu/\rho)_i$), where, w_i, is the proportion by weight; and $(\mu/\rho)_i$ mass attenuation coefficient of the i^{th} element.

2.2 Ratio method

The μ/ρ of the organic compounds are obtained using mixture rule. They are further utilized to

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Table 1 – Elemental composition of organic compounds

Compounds	Formula	Weight fraction (w_i)	<Z>	$Z_{eff, XmuDat}$	$Z_{eff, PL}$	
					X=2.94	X=3.50
Glucose	$C_6H_{12}O_6$	H: 0.0667; C: 0.4000; O: 0.5333	4.00	7.08	7.01	7.08
Ethanol	CH_3CH_2OH	H: 0.1317; C:0.5214; O:0.3469	2.89	6.79	6.61	6.69
Acetic acid	CH_3COOH	H: 0.0671; C: 0.4000; O:0.5329	4.00	---	7.09	7.15
Trichloroethylene	C_2HCl_3	H:0.0077; C:0.1828; Cl: 0.8095	10.67	15.96	15.62	15.82
Chloroform	$CHCl_3$	H: 0.0084; C: 0.1006; Cl:0.8909	11.60	16.4	22.90	21.83
Benzene	C_6H_6	H: 0.0774; C: 0.9226	3.50	5.74	5.83	5.86
Acetone	C_3H_6O	H: 0.1041; C: 0.6204; O:0.2755	3.20	6.39	6.42	6.51
Phenol	C_6H_5OH	H: 0.0638; C: 0.7604; O: 0.1758	3.85	---	6.23	6.30
Chlorobenzene	C_6H_5Cl	H: 0.0448; C:0.6403; Cl:0.3149	4.83	12.16	11.58	12.17
Naphthalene	$C_{10}H_8$	H: 0.0629; C: 0.9371	3.78	5.79	5.89	5.90
Adenine	$C_5H_5N_5$	H: 0.0373; C: 0.4444; N: 0.5183	4.67	6.45	6.51	6.53
Alanine	$C_3H_7NO_2$	H: 0.0792; C:0.4044; N:0.1572 ; O:0.3592	3.69	6.78	6.89	6.95
Anthracene	$C_{14}H_{10}$	H: 0.0567; C:0.9435	3.92	5.81	5.90	5.92
Carbon Tetrachloride	CCl_4	C:0.0781; Cl: 0.9219	14.80	16.61	16.38	16.47
Diethyl Either	$(C_2H_5)_2O$	H: 0.1359; C:0.6482; O: 0.2159	2.80	6.15	6.31	6.40
Sucrose	$C_{12}H_{22}O_{11}$	H: 0.0648; C:0.4211; O:0.5142	4.04	7.00	7.09	7.15

compute the molecular cross-section, σ_m; atomic cross-section, σ_a; electronic cross-section, σ_e; electronic cross-section, σ_e; and effective atomic number, Z_{eff} by following equations:

$$\sigma_m = \frac{\left(\mu/\rho\right)\left(\sum_i n_i A_i\right)}{N} \quad \ldots (1)$$

$$\sigma_a = \frac{\sigma_m}{\sum_i n_i} \quad \ldots (2)$$

$$\sigma_e = \frac{1}{N}\sum_i \frac{f_i A_i}{Z_i}\left(\mu/\rho\right)_i \quad \ldots (3)$$

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad \ldots 4)$$

where, N is Avogadro's number in atom g^{-1}; A_i and Z_i are atomic weight and atomic number of the i^{th} element present in the organic compound, respectively; n_i is the number of atoms of the i^{th} element present in a organic compound, e.g., C_6H_5OH; the number of carbon atoms, n_1=6; number of hydrogen atoms, n_2=6; number of oxygen atom, n_3= 1; and $\sum_i n_i = 13$. Also, f_i is the fractional abundance of the i^{th} element, $n_i / \sum_i n_i$, e. g., in C_6H_5OH, the fractional abundance of carbon atom, 6/13= 0.4615; $(\mu/\rho)_i$ is the mass attenuation coefficient of the i^{th} element present in a organic compound.

2.3 Direct method

Computation of the effective atomic number by direct method, Z_{Pleff} for the organic compounds is calculated using practical formula[9]. The Z_{Pleff} of the organic compounds is calculated using Eq. (5):

$$Z_{Pleff} = \frac{\sum_i f_i A_i \left(\mu/\rho\right)_i}{\sum_j f_j \frac{A_j}{Z_j}\left(\mu/\rho\right)_j} \quad \ldots (5)$$

where, the ratio A/Z between the atomic mass and the atomic number is approximately constant.

2.4 Auto-Z_{eff} method

Auto-Z_{eff} is user-friendly computer software in Visual Basic for rapid computation of the energy dependent effective atomic numbers. In this method, effective atomic number is determined via exploitation of the smooth correlation between atomic cross-section and atomic number. The cross-section values are contracted with the cross-section matrix as a function of Z, and an effective Z for energy is obtained by interpolation of Z values between adjacent cross-section data[10].

2.5 Interpolation method

The μ/ρ values of the organic compound are derived using mixture rule. The attenuation cross-section of the organic compounds is calculated using Eq. (6):

$$\sigma_{compound} = \frac{\left(\mu \frac{[...]}{\rho}\right)_{compound}}{N \sum_i \left[\left(\frac{w_i}{A_i}\right)\right]} \quad \ldots (6)$$

where, N is Avogadro's number in atom g^{-1}; w_i, is weight fraction of the i^{th} element in a organic compound; and A_i is the atomic weight of the i^{th} element in a organic compound; w_i and A_i are dimensionless quantities. The attenuation cross-section values obtained are logarithmically interpolated to compute the effective atomic numbers using following Eq. (7):

$$Z_{eff,IL} = \frac{Z_1\left(\log\sigma_2 - \log[\sigma) + Z_2(\log\sigma - \log[\sigma_1)]\right]}{\log\sigma_2 - \log\sigma_1} \quad \ldots (7)$$

where, σ_1 and σ_2 are the cross-sections of element in between which the atomic cross-section σ of the organic compound lies; and Z_1 and Z_2 are atomic numbers of the elements corresponding to the cross-sections σ_1 and σ_2, respectively.

2.6 Power Law method

The effective atomic number using power law, $Z_{eff,PL}$ of an organic compound is calculated using the following Eq. (8)[12]:

$$Z_{eff,PL} = \sqrt[x]{a_1 Z_1^x + a_2 Z_2^x} + \quad \ldots (8)$$

where, $a_i = \frac{n_i(Z_i)}{\sum_i n_i(Z_i)}$; $a_1, a_2, \ldots$, are the fractional contents of electrons belonging to element Z_1, Z_2, ……, respectively; n_i, is the number of electrons in one mole belonging to each element Z_i. The x values are in range 2.94 - 3.5[18,19].

2.7 XmuDat method

XmuDat computer program is a single-valued effective atomic number for a organic compound[13]. The XmuDat uses the following Eq. (9):

$$Z_{eff,XmuDat} = \left(\sum_i [\alpha_i Z_i^{m-1}\right)^{\frac{1}{m-1}}] \quad \ldots (9)$$

where, α_i is the fractional number of the electrons of the element; and m is a constant between 3 and 5. Here, data source for XmuDat is from Hubbell and Seltzer[20].

2.8 Kerma

The Kerma is defined as the initial kinetic energy of all secondary charged particles liberated per unit mass at a point of interest by uncharged radiation[21,22]. It is applicable to photons (x-ray, gamma ray, bremsstrahlung, etc) and neutrons; and has the same unit J kg^{-1} = Gy, as the absorbed dose. The Kerma of the organic compounds relative air is derived by Eq. (10):

$$K_a = \frac{K_{Compound}}{K_{Air}} = \frac{\left(\mu_{en}/\rho\right)_{Compound}}{\left(\mu_{en}/\rho\right)_{Air}} \quad \ldots (10)$$

The mass energy-absorption coefficient, μ_{en}/ρ of the organic compounds are calculated using mixture rule ($(\ _{en}/\ ) = \sum_i^n w_i (\ _{en}/\ )_i$), where w_i and $(\mu_{en}/\rho)_I$, are the weight fraction and the mass energy-absorption coefficient of the i^{th} element of the compounds. The values of $(\mu_{en}/\rho)i$ are taken from the NIST data[20].

3 Results and Discussion

The variation of mass attenuation coefficients, μ/ρ of the organic compounds with photon energy is shown in Fig. 1. The effective atomic numbers of the organic compounds are shown in Figs 2 (a-e). The effective atomic numbers using XmuDat, power law and average methods are given in Table 1. The comparison of the different methods along with experimental data for glucose and alanine is shown in Figs 3 (a-b). The variation of Kerma relative to air with photon energy of the organic compounds is shown in Fig. 4.

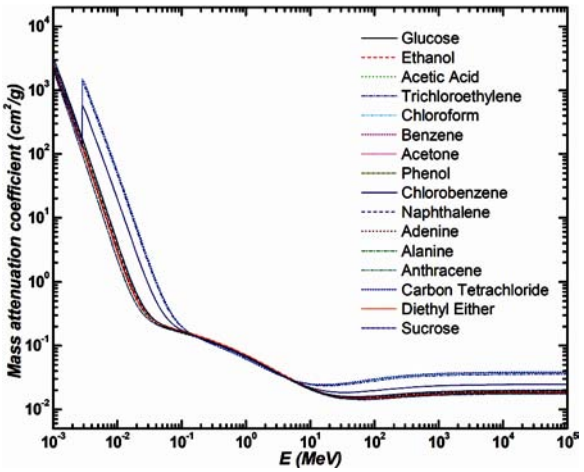

Fig. 1 – Mass attenuation coefficients of organic compounds

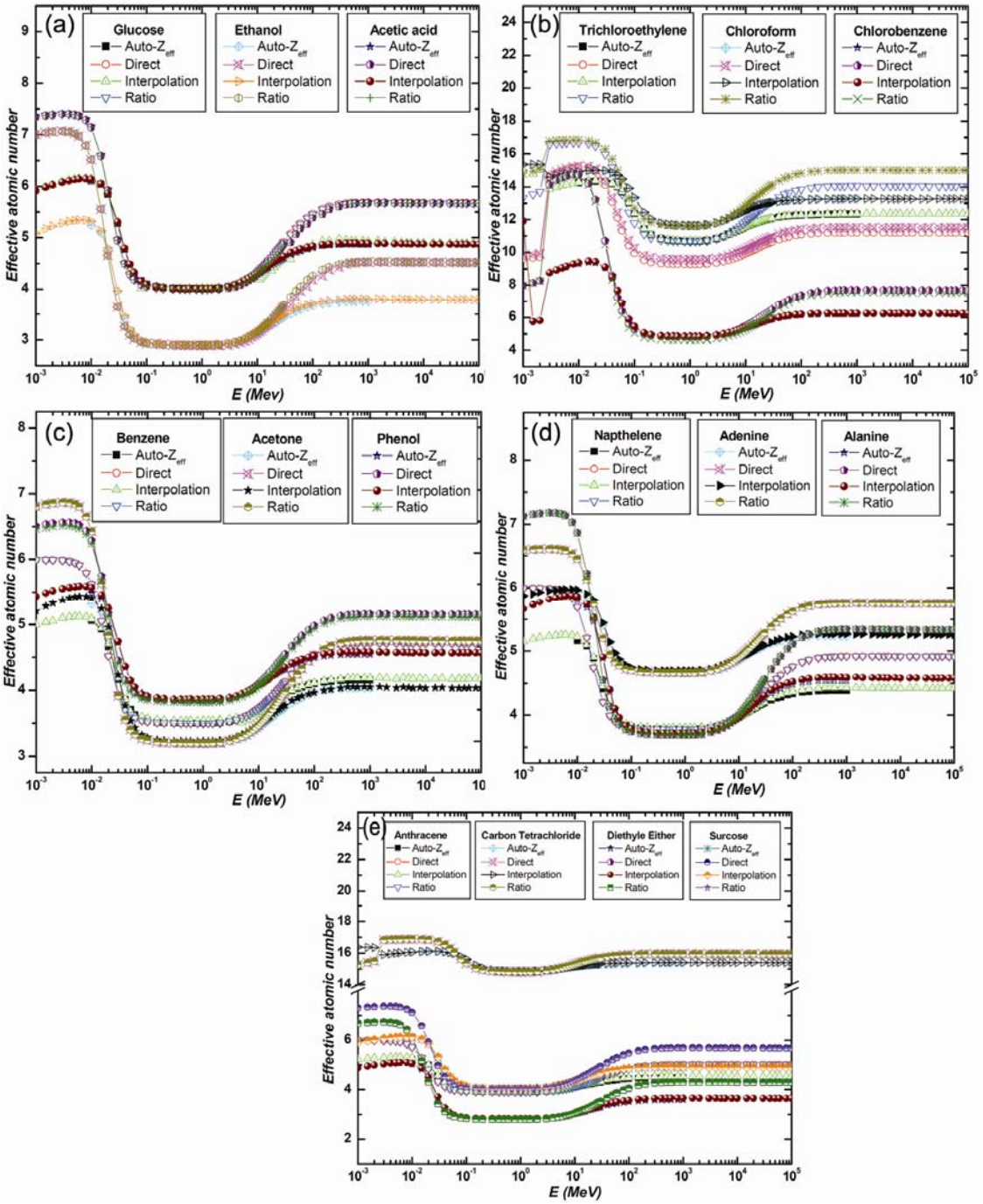

Fig. 2 – Effective atomic numbers of the organic compounds

3.1 Mass attenuation coefficients

Variation of mass attenuation coefficients, μ/ρ of the selected organic compounds with photon energy is shown graphically in Fig. 1 for photon energy region 1 keV - 100 GeV. It is to be noted that the μ/ρ values of the organic compounds decrease rapidly with photon energy up to 100 keV for trichloroethylene, chloroform, chlorobenzene and carbon tetrachloride, whereas up to 50 keV for the remaining. It is found that the μ/ρ values of trichloroethylene, chloroform and carbon tetrachloride are almost same. As photon energy increases, the μ/ρ value decreases slowly for all the compounds up to 10 MeV and beyond it again gradually increase and become independent above 100 MeV. This variation can be explained by partial photon interactions namely photoelectric absorption,

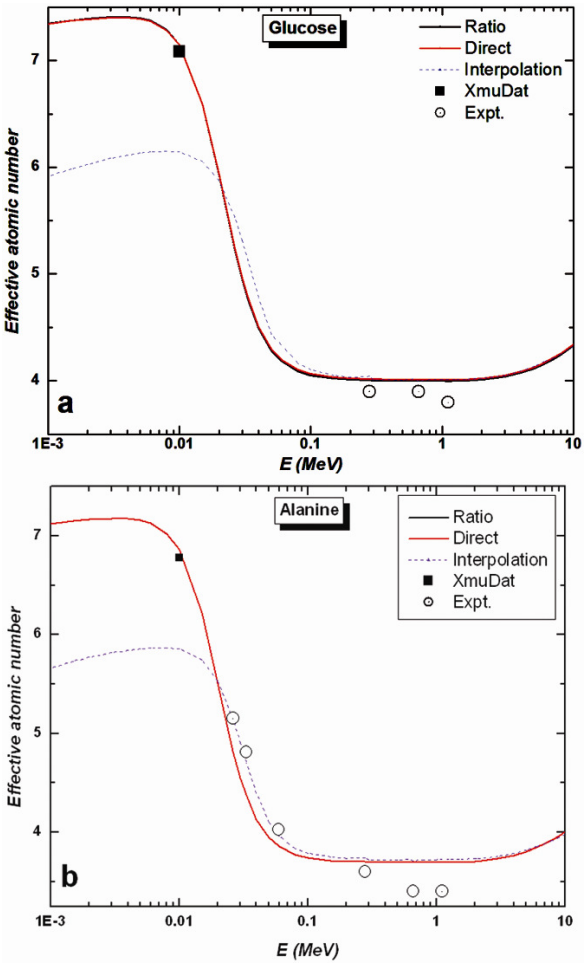

Fig. 3 – Comparison of XCOM effective atomic numbers with experimental data

Compton scattering and pair production, which are dependent upon photon energy (E) and atomic number (Z).

Sharp decrease in μ/ρ values below 50 keV can be explained on the basis of the dominant photoelectric absorption effect, where photon interaction cross-section depends on Z^4 (for low energy) and Z^5 (for high energy) and photon energy as $E^{-7/2}$. Above 50 keV, the Compton scattering process replaces photoelectric effect, where photon interaction cross-section varies linearly with Z and E^{-1}; thus, the μ/ρ values of the organic compounds decrease. In the pair production region, the interaction cross-section depends on Z^2 and log E; and hence, the μ/ρ values increase slowly and become independent. It is found that μ/ρ values of trichloroethylene, chloroform, chlorobenzene and carbon tetrachloride are having a peak at 2.822 keV due to k-absorption edge of chlorine.

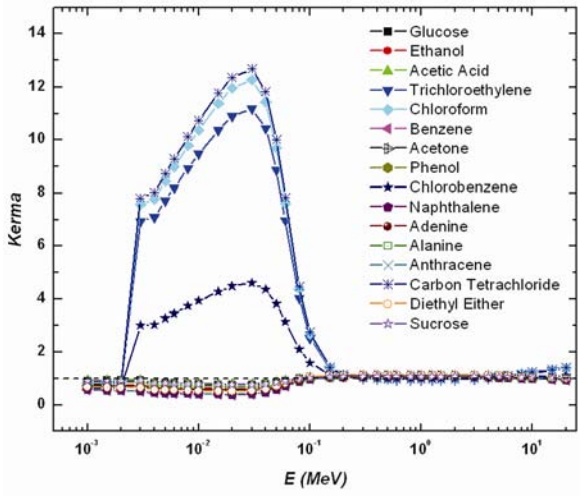

Fig. 4 – Kerma relative to air of organic compounds

3.2 Effective atomic numbers

Effective atomic numbers of the organic compounds using different methods is shown in Figs 2 (a-e). From Figs 2 (a-e), it is clear that the values computed by Auto-Z_{eff}, direct, logarithmic interpolation and ratio are in good agreement in intermediate energy region where the Compton scattering dominates. A significant difference in the effective atomic numbers of the organic compounds is noted for typically low ($10<E<50$ keV) as well as high energies ($E>10$ MeV).

It is found that the effective atomic numbers of all the organic compounds by the Auto-Z_{eff} with logarithmic interpolation and the ratio with direct methods are in very good agreement. In low energy region (1 - 10 keV), there is large difference in effective atomic number values using these methods [Figs 2 (a-e)]. Therefore, experimental data in low photon energy region are required to establish the appropriate method.

From Figs 2 (a-e) and Table 1, it is to be noted that the effective atomic numbers of all the organic compounds in intermediate energy region (50 keV $<E<$10 MeV) are approximately equal to average atomic number using the chemical formula $\langle Z \rangle = \frac{1}{n} \sum_i n_i Z_i$. The independency of the effective atomic numbers in Compton scattering region are reported for photon energy range 54 - 1333 keV[3,23,24]. From this analysis, it is concluded that Auto-Z_{eff}, direct, logarithmic interpolation and ratio methods are applicable in intermediate energy (50 keV $< E <$10 MeV) for computation of effective atomic numbers.

From Table 1, it is to be noted that the effective atomic numbers using the XmuDat and power law

methods are very close to each other. The average effective atomic number of the organic compounds (given in Table 1) is equivalent to Auto-Z_{eff}, direct and interpolation in intermediate energy region.

The theoretical values are compared with experimental data for glucose and alanine as shown in Figs 3 (a-b). Hence, it can be concluded that theoretical methods, viz., Auto-Z_{eff}, direct, logarithmic interpolation and ratio are appropriate in intermediate photon energy region.

3.3 Kerma

The Kerma relative to air, K_a values of the organic compounds are plotted as a function of photon energy (1 keV to 20 MeV) in Fig. 4. The variation of K_a with photon energy represents variation of effective atomic numbers and so can be explained in similar manner. The organic compounds containing ^{17}Cl are showing comparatively high K_a values. It is to be noted that the K_a values of the CCl_4 (92.19% Cl) reaches up to 12.68 at 30 keV. It is found that the K_a values of all the compounds reach a constant value (~unity) beyond 200 keV and up to 10 MeV.

3.4 Uncertainties

The uncertainties in μ/ρ is about 1% for low-Z ($1<Z<8$) percent in Compton region (30 keV - 100 MeV). Below 30 keV, energy uncertainties are as much as 5-10% because of: (i) correction to experiments for high-Z impurities; and (ii) departure from Compton cross-section from Klein-Nishina theory. Also, above 100 MeV energy, uncertainties in μ/ρ may be 5-10%[25]. Uncertainties in photon energy absorption coefficient may have slightly greater values. Computations of effective atomic number using Auto-Z_{eff} are of order of 1-2% in the photon energy region 10 keV-100 MeV. The computation of effective atomic numbers is not attempted for photon energy down to 1 keV, where an uncertainty ranges up to 25-50%[10].

4 Conclusions

The effective atomic numbers of dosimetric interest organic compounds are calculated by various methods and compared with experimental data. Auto-Z_{eff}, direct, logarithmic interpolation and ratio methods are applicable in intermediate photon energy where Compton scattering is dominant. Effective atomic numbers calculated using power law and XmuDat are found very close to each other. The Kerma of the organic compounds relative to air is dependent upon photon energy and chemical compositions.

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