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RESEARCH ARTICLE

Investigation of the Mass Attenuation Coefficients, Effective Atomic Numbers and Electron Densities for Compounds of Painkiller

Tekerek Saniye*

Sutçu Imam Üniversity, Kahramanmaraş, Turkey

ABSTRACT

In this study the effects of gamma radiations with compounds are an important subject in the field of medicine, radiation shielding and radiation physics. With technological advances the using of radiation has increased in the medicine in the last century. The mass absorpsion coefficient (μ/ρ) is the fundamental a quantity characterizing gamma ray and is of major importance in radiation shielding. In this study, the mass absorption coefficient of painkillers named Ketoprofen, Flurbiprofen, Etodolac, Ibuprofen, Meloxicam, Diclofenac and Aspirin were calculated at energy range from 4.65 keV to 59.543 keV using the WinXCom data programme. In addition total atomic (σta), moleculer (σtm), electronic cross-section (σte), effective atomic number (Zeff), effective electron density (Neff) were calculated.

INTRODUCTION

With the increasing use of radiation sources in areas related to human health such as nuclear medicine, radiotherapy and radiology, it was necessary to examine the parameters that are considerable in the interaction of photon with material. In radiation dose calculations, the effective atomic number information of the samples absorption of beam in the samples were required [1,2]. The mass absorption coefficient, which is a characteristic feature for materials is a very significant parameter in agriculture, pharmacy, radiation dosimetry, biology, nuclear and radiation physics [3]. The accurate reliable values of mass attenuation coefficients were required to provide essential data in varied fields such as nuclear diagnostics, radiation protection, nuclear medicine, radiation biophysics and etc. [4]. The effective atomic number physically enables the characteristic of the compound to be understandable with the help of a single atomic number [5]. μ/ρ was also used to calculate and control the material thickness because radiation can change the characteristics of material. Since this may cause various undesirable results, it was very important to examine the interaction of many materials, alloys and compounds with radiation and to know what changes they cause in the material [6]. In the literature, the effects of radiation material interactions at different energies on Z_{eff} and N_{eff} were studied. Z_{eff} were calculated in the energy range of 15.746-40.930 keV using the mixing rule depending on the Ni contribution in CuCoNi alloys, and it was stated that the Z_{eff} value increased with the increase in Ni ratio [7]. Z_{eff} and N_{eff} between at various energies of essential amino acids were calculated theoretically [8]. The Z_{eff} of composite materials at various energy ranges of 280 to 1115 keV were obtaned [9]. Experimental and theoretical μ/ρ values of vitamins

***Corresponding author**

Tekerek Saniye, Vocational School of Health Services, Sutçu Imam Üniversity, Kahramanmaraş, Turkey

E-mail: saniyetekerek@ksu.edu.tr

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in some photon energies were calculated [10]. The mass attenuation coefficient for compounds or compositions was calculated with the help of WinXCom program. WinXCom is a data programme base the "mixing rule". In this rule, the elements in the ingredient are considered independent from each other and their interaction with each other is neglected [11].

In this present work were calculated the mass attenuation coefficients for some painkiller compounds such as Ketoprofen ($C_{16}H_{14}O_3$), Flurbiprofen ($C_{15}H_{13}FO_2$), Etodolac ($C_{17}H_{21}NO_3$), Ibuprofen ($C_{13}H_{18}O_2$), Meloxicam ($C_{14}H_{13}N_3O_4S_2$), Diclofenac ($C_{14}H_{11}Cl_2NO_2$) and Aspirin ($C_9H_8O_4$) in the energy range from 4.65 keV to 59.543 keV using the WinXCom data. Z_{eff} and N_{eff} parameters were calculated with the help of the data obtained. It has been observed that N_{eff} and Z_{eff} values are interrelated and parallel to each other. The computational results of the pain relief compounds μ/ρ, Z_{eff} and N_{eff} presented in this study can be referenced as guiding in a variety of medical applications and fields. In the paper, calculated datas were published on the study of mass attenuation coefficient calculate on painkiller compounds in the photon energy 4.65 to 59.543 keV through which radiation interaction of the drug can be defined.

MATERIAL AND METHODS

The substances used in around the world to address various pains are listed in table 1. Use of aspirin, ibuprofen were said to show beneficial synergistic effects by combatting pain at multiple sites of action [12]. *Flurbiprofen was used in the treatment of pain or inflammation in humans. Flurbiprofen is indicated for the management of excimer laser photorefractive keratectomy, and ocular gingivitis. Recent reports suggest use of flurbiprofen in radioprotection, the inhibition of colon tumor, the protection of post irradiation myelosuppression and peridontal surgery [13]. Etodolac drug is an effective drug in the treatment of osteoarthritis, rheumatoid arthritis and spinal rheumatism.* Since these painkillers was used for different purposes in the field of medicine [14]. It was considered necessary theoretically to examine their reactions to high energy rays.

The μ/ρ for a compound material is the total of the mass attenuation coefficients of every element according to "mixing rule" [15]. According to the WinXcom program, μ/ρ is calculated with the help of formula (1).

$$\left(\frac{\mu}{\rho}\right)_c = \sum_i \omega i \left(\frac{\mu}{\rho}\right)_i \quad (1)$$

In equation (1), ω_i is fractional weight of the i atom.

Theoretical μ/ρ is calculated for compound materials using the WinXcom. Using the equation (2) σ_{tm} values were calculated [16].

$$\sigma_{tm} = \frac{1}{N_A}\left(\frac{\mu}{\rho}\right)_C \sum_i n_i A_i \quad (2)$$

A_i is the atomic weight, n_i is the number of atoms, N_A is Avogadro's number.

σ_{ta} is calculated using the following Equation (3) [16].

$$\sigma_{ta} = \frac{\sigma_{tm}}{\sum n_i} \quad (3)$$

In formula (3), σ_{ta} is the total atomic cross section, σ_{tm} is the total molecular cross section, n_i is the total number of atoms. The unit of σ_{ta} is cm^2/atom.

The electronic cross section was obtaned by using the mass attenuation coefficient of each element in the samples. σ_{te} was calculated using Formula (4) [16].

$$\sigma_{te} = \frac{1}{N_A}\sum_i f_i \frac{A_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i ; \qquad f_i = \left(\frac{n_i}{\sum_i n_i}\right) \quad (4)$$

Z_i atomic weight and f_i is abundance fraction.

Z_{eff} was calculated using formula (5) [5].

$$Z_{eff} = \frac{\sigma_{ta}}{\sigma_{te}} \quad (5)$$

N_{eff} was calculated using the following formula (6) [17].

$$N_{eff} = \frac{N_A \; n_{tot} Z_{eff}}{\sum_i n_i A_i} \quad (6)$$

Table1: Painkiller coumpounds.

Ketoprofen	$C_{16}H_{14}O_3$
Flurbiprofen	$C_{15}H_{13}FO_2$
Etodolac	$C_{17}H_{21}NO_3$
İbuprofen	$C_{13}H_{18}O_2$
Meloxicam	$C_{14}H_{13}N_3O_4S_2$
Diclofenac	$C_{14}H_{11}Cl_2NO_2$
Aspirin	$C_9H_8O_4$

RESULTS AND DISCUSSION

WinXCom program determines the μ/ρ of the compounds consisting of more than single element for any sample, taking into account "mixture rule" while calculating the mass absorption coefficients. According to the this rule, μ/ρ of the compound is the sum of the mass absorption coefficients of each element [18]. μ/ρ, Z_{eff} and N_{eff} values calculated at the specified energies of the compounds are given in tables 2-4.

Table 2: The mass attenuation coefficients μ/ρ (cm^2/gr) for painkiller compounds at different photon energies.

Compounds	4.65 keV	5.9 keV	8.1 keV	12.2 keV	30.2 keV	59.543 keV
$C_{13}H_{18}O_2$	27.33	13.28	5.11	1.579	0.282	0.191
$C_{17}H_{21}NO_3$	28.84	14.01	5.388	1.656	0.284	0.189
$C_{16}H_{14}O_3$	29.29	14.23	5.468	1.667	0.282	0.187
$C_{15}H_{13}FO_2$	31.7	15.44	5.941	1.813	0.290	0.187
$C_9H_8O_4$	35.48	17.28	6.643	2.011	0.301	0.188
$C_{14}H_{13}N_3O_4S_2$	104.3	53.56	21.71	6.686	0.618	0.228
$C_{14}H_{11}Cl_2NO_2$	134.8	70.37	28.93	9.009	0.782	0.248

Table 3: The effective atomic number (Z_{eff}) for painkiller compounds at different photon energies.

Compounds	4.65 keV	5.9 keV	8.1 keV	12.2 keV	30.2 keV	59.543 keV
$C_{13}H_{18}O_2$	6.510	6.470	6.333	5.861	4.006	3.524
$C_{17}H_{21}NO_3$	6.600	6.567	6.454	6.055	4.303	3.804
$C_{16}H_{14}O_3$	6.611	6.590	6.505	6.157	4.675	4.186
$C_{15}H_{13}FO_2$	6.853	6.838	6.759	6.446	4.829	4.278
$C_9H_8O_4$	7.031	7.017	6.954	6.700	5.213	4.641
$C_{14}H_{13}N_3O_4S_2$	11.899	12.051	12.163	12.247	8.732	5.963
$C_{14}H_{11}Cl_2NO_2$	13.503	13.687	13.818	13.672	10.045	6.396

Table 4: The effective Electron Density ($N_{eff}x10^{23}$) (electron/gram) for painkiller compounds at different photon energies.

Compounds	4.65 keV	5.9 keV	8.1 keV	12.2 keV	30.2 keV	59.543 keV
$C_{14}H_{11}Cl_2NO_2$	8.234	8.347	8.427	8.337	6.125	3.900
$C_{14}H_{13}N_3O_4S_2$	7.339	7.432	7.501	7.553	5.385	3.678
$C_{13}H_{18}O_2$	6.269	6.232	6.099	5.647	3.859	3.395
$C_{17}H_{21}NO_3$	5.807	5.778	5.679	5.328	3.786	3.347
$C_{16}H_{14}O_3$	5.164	5.148	5.082	4.808	3.653	3.277
$C_{15}H_{13}FO_2$	5.236	5.224	5.164	4.925	3.689	3.269
$C_9H_8O_4$	4.934	4.924	4.880	4.701	3.658	3.257

As can be seen from the table 2, with increasing energy a decrease is observed in the μ/ρ values and accordingly the Z_{eff} values. The highest mass absorption coefficient of 134.8 belongs to the compound $C_{14}H_{11}Cl_2NO_2$ called Diclofenac at 4.65 keV energy. The mass attenuation coefficient value of $C_{14}H_{11}Cl_2NO_2$ compound named Diclofenac was found as 0.248 at the highest energy calculated at 59.543 keV. It can be seen from Table 2 that the lowest mass attenuation coefficient of the calculated energy ranges belongs to the $C_{13}H_{18}O_2$ compound.

It seems obvious that the total moleculer cross-section values decrease with increasing photon energies as shown in the figure 1. It can be seen from figure 1 that the lowest total moleculer cross-section value of the calculated energy ranges belongs to the İbuprofen $C_{13}H_{18}O_2$ compound.

It is clearly seen that the mass attenuation coefficient depends on the photon energy and on the chemical structure of the compounds. The μ/ρ values decrease with increasing photon energies as shown in the table 1. With the presence of Cl in the compound, Diclofenac ($C_{14}H_{11}Cl_2NO_2$) compound has the largest Z_{eff} value. Simultaneously while the effective atomic number for the $C_{14}H_{11}Cl_2NO_2$ compound increased, a parallel increase was observed in the effective electron density. Although there is not much change in low energies in compounds with multiple elements, a decrease in the effective atomic numbers has been observed due to the increase in energy. Ibuprofen ($C_{13}H_{18}O_2$) is a pain reliever with the lowest mass attenuation coefficient in the energies studied. In general, as the number of quantity elements forming the compound increases, μ/ρ and Z_{eff} values increase.

The effective electron dentisity value of $C_{14}H_{11}Cl_2NO_2$ compound named Diclofenac was found as 3.900 at the highest energy calculated at 59.543 keV. It can be seen from table 4 that the lowest effective electron dentisity value of the calculated energy ranges belongs to the $C_{13}H_{18}O_2$ compound.

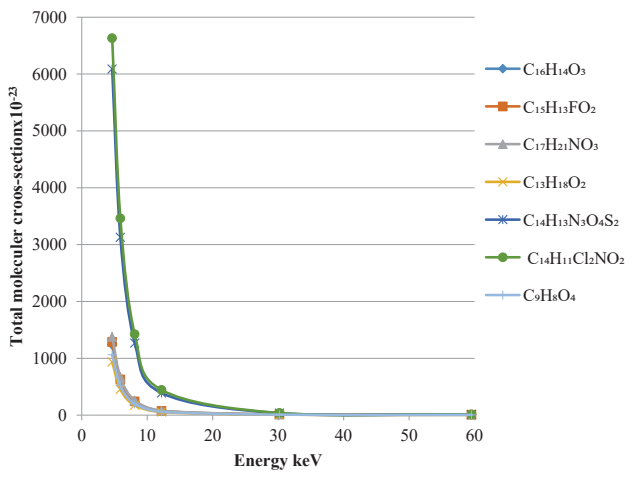

Figure 1 Total moleculer cross-section for painkiller compounds at different photon energies.

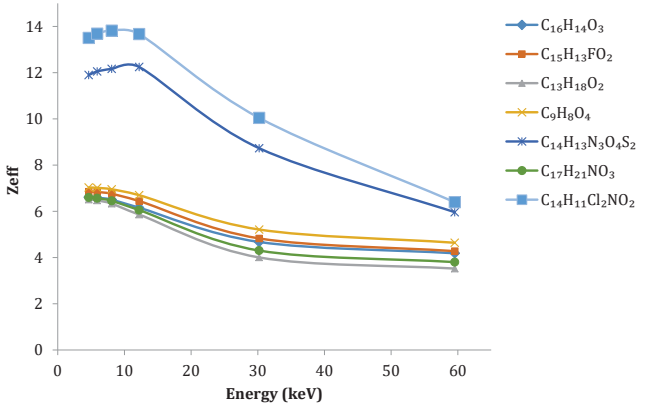

Figure 2 Effective atomic number for painkiller compounds at different photon energies.

RESULTS

In this study, μ/ρ at various energies were calculated for some compounds belonging to painkillers. By using μ/ρ values, σ_{tm}, σ_{ta}, σ_{te}, Z_{eff}, N_{eff} values were calculated. Absorption of the photon at various energies occurs depending on the properties of the material under study. Therefore, beam permeability data at different energies provide information about the absorption and shielding properties of the material. Radiation absorption properties at low energies give better results for pain relief compounds. As can be seen from the results of the calculations, the radiation energy and the mass absorption coefficient vary, and it is understood that the materials cause changes in the attenuation parameters of the material withal increasing radiation. The data obtained from this study is important in terms of guiding researchers working in this field. The data obtained in the light of these values will be used in various fields and it is thought to be suitable for use as shielding material in order to protect from radiation in low and medium energy beams.

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