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Measurement of Total Electronic Cross-Section, Total Atomic Cross-Section, Effective Atomic Numbers, Effective Electron Densities and Kerma for Some Br Compounds

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ABSTRACT

The aim of this study is to calculate the experimental and theoretical the mass attenuation coefficient some Br compounds by using transmission method. Also using these values were determined the total electronic section, total atomic section, effective atomic number, effective electron density and Kerma. We performed the calculations of these values in attenuation by using direct excitation experimental geometry. The total attenuation cross sections of some halogene Br compounds were measured in a narrow beam good geometry using a high resolution Si(Li) detector in the energy with γ photons at 59.543 keV from Am-241 annular source. Theoretical mass attenuation coefficient values were computed from the XCOM data programme, based on mixture rule method. This study provide new insight into the literature since the values of effective atomic number, electron density and Kerma for some Br compounds have not been determined before. According to the results shown in mass attenuation coefficient, Z_{eff} and N_{eff} of Br compounds are closely associated with chemical structure. This research were undertaken to explore how Bromine compounds is gamma ray shielding material.

INTRODUCTION

Defining the interplay between radiation and matter, mass attenuation coefficient have been widely used in the field of interaction of photon. While penetrating the compounds, the intensity of gamma photon reduces and mass attenuation coefficient measures the energy absorbed by the compounds. The gamma transmission method is used for measurement of photon atomic emission parameters. The mass attenuation coefficient depends on the atomic number of element and the chemical structure [1].

The mass absorption coefficients of materials are important in several applications of medical physics, nuclear physics, radiation shielding, radiotherapy, medical fields. Theoretically mass attenuation coefficient of compounds calculated by Bragg's mixture rule [2], which represent that the total mass attenuation coefficient of any compound is the sum of fractional weighted of the individual elements. By using Lambert's law and the rule of mixture, we can obtain to determine theoretically the mass attenuation coefficient. The correct experimental mass attenuation coefficient values are essential to determine exact effective atomic number.

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For compounds has been called as effective atomic number Z_{eff}, suggested. Also scientists was created theoretical expressions to evaluate effective atomic numbers for the separate photon interaction processes [3,4]. The experimental Z_{eff} and N_{eff} values are crucial for many fields. The electron density is formulates as the numbers of electrons per unit mass. In addition, effective atomic number and the electron density have a physical meaning that depends on the chemical structure. A large body of literatüre has determined the data of this parameter for different materials [5-8]. To understand the chemical structure, physical and biological properties of a compound, the knowledge of effective atomic number is crucial [9,10]. The tables of mass attenuation coefficient were published for element, mixture and compounds at various energy [11].

Photons interact with matter and lose their energy as a result of the three main processes which are, photoelectric effect, Compton scattering and pair-production. The attenuation coefficient is a measure of the average number of interactions between incident photon and matter that occur in a given mass per unit area thickness of the compounds encountered. The mass attenuation coefficient (μ/ρ) is an event dependent on the possibility of photon interaction with compound samples. The attenuation of gama rays are involved where the intensity is reduced to I after the photon beam of intensity I_0 the passes through compound of mass per unit area thickness (t).

Also another important parameter calculated is Kerma. Kerma is kinetic energy released in air. In other words, Kerma is the kinetic energies of charged ionizing particules liberated by radiation. The numerical value of the kerma have defineted that of the absorbed dose [12,13]. The availability of accurate Kerma value is significant in dosimety and medical therapy. This study has been used in Bromine compounds and is important because of its wide use in applied fields such as radiation physics, health physics and medicine [14]. The purpose of this study is to determine molecular, atomic and electronic cross-section, effective atomic numbers, effective electron density for experimental measurement and theoretical calculated of Kerma by using mass attenuation coefficient for some compounds of bromine.

Bromides are used as anticonvulsants in both veterinary and human medicine [14]. There are various kinds of bromides but in this study some particular bromides were taken into consideration. $CaBr_2$ is an component in medication and food preservatives. The Sodium Bromide (NaBr) is used as a microbiocide in water treatment. Also known as sedoneural, sodium bromide has used in pharmaceutical as sedative. Sodium bromide is been used one of as antiepileptic drugs due to properties. Potassium bromide is used to strengthen the dough as a dough puff in bread making [15]. The CuBr compound is used in food packaging [16]. $KBrO_3$ (Potassium Bromate) is used as a chemical in hair products, and it is a food additive used for the brewing of beer. $KBrO_3$ has been used in bread making process [17-20]. $C_{19}H_{10}Br_4O_5S$ (Bromophenol Blue) is a dye [21]. C_6H_6BrN (4-Bromoaniline) is employed as the pharmaceutial [22]. $C_{21}H_{16}Br_2O_5S$ (Bromocresol Purple) is applied in laboratories to measure albuminin the blood [23]. In microbiology laboratory, it is used for staining dead cells and for the assaying of lactic acid bacteria [24].

The effective atomic number is a physical parameter informing us abouth the caracteristic properties of Br compounds. This paper presents the experimental measurement and theoretically calculate of the effective atomic numbers, effective electron density, molecular cross-section, atomic cross-section, electronic cross-section and Kerma for some Br compounds. Our present investigation of mass attenuation coefficients (μ/ρ) of some Br compounds for total photon interaction processes will generate fresh insight in to the field, since the response of medically used bromine compounds to radiation has not been studied before.

Theory

Theoretical procedures were applied to the data obtained as a result of the experiment. The molecular cross section, atomic cross section, effective atomic number and effective electron density can be determined using experimental results of the mass attenuation coefficients. The effective atomic number (Z_{eff}) are calculated [25-27] as the ratio of atomic cross section (σ_{ta}) to electronic cross section (σ_{te}) i.e. The following formulas described were used to calculations of the results.

Values of mass attenuation coefficients are then used to determine the total molecular cross section σ_{tm} by the following relation [28].

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

where $\sum_i n_i A_i$ is the molecular weight, A_i is the atomic weight of the ith element in a compound, n_i is the number of atoms of the element in a compound. N_A is Avogadro's number. Total mass attenuation coefficient is calculated by following equation [29].

$$\frac{\mu}{\rho} = \frac{1}{\rho x} \mathrm{In}\left(\frac{I_0}{I}\right); \rho x = \frac{m}{\pi r^2}$$

where (I) with absorber count incident photon, and (I_0) without absorber count transmission photon intensity, ρ is the density of the material, x is the thickness of the sample (cm^{-1}). ρx is the mass per unit area of the sample (g/cm^2). Where m is the mass of the sample (g) and r is the radius of the compound powder sample (cm).

The equation below is particularly useful in calculating the total atomic cross section σ_{ta} [28]:

$$\sigma_{ta} = \frac{\sigma_{tm}}{\sum n_i}$$

where σ_{ta} the total atomic cross section, total molecular cross section σ_{tm}, n_i, total number of atoms in a compound, the total electronic cross section σ_{te} for the individual element is expressed by the following formula [28]:

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

f_i; the fractional abundance of element i with respect to the number of element.

A_i is the atomic weight and Z_i is the atomic number of element of the constituent element i, respectively.

The total atomic and electronic cross sections are closely to the effective atomic number (Z_{eff}) through the following relation formula [28]:

$$Z_{eff} = \frac{\sigma_{ta}}{\sigma_{te}}$$

The effective electron number or electron density, N_{eff} can be derived from the formula [29] below:

$$N_{eff} = \frac{\left(\mu/\rho\right)_c}{\sigma_{te}} = \frac{N_A n_{tot} Z_{eff}}{\sum_i n_i A_i}$$

where; $\left(\mu/\rho\right)_c$ is compounds mass attenuation coefficient and σ_{te} is the total electronic cross section.

Kerma is the product of the air mass attenuation coefficient and the compounds mass attenuation coefficient. Kerma of an compounds relative to air can be calculated as [30]:

$$\text{Kerma} = \frac{\left(\mu/\rho\right)_{compounds}}{\left(\mu/\rho\right)_{air}}$$

In here; $\left(\mu/\rho\right)_{compounds}$ is mass attenuation coefficient of compounds and $\left(\mu/\rho\right)_{air}$ is air mass attenuation coefficient.

Experimental detail

Total mass attenuation coefficients were measured through transmission with narrow beam geometry method. It is a fact that gamma attenuation information dependent on photon energy is required for material characterization of compounds. In the present experiment, a Si(Li) detector with multi channel analyzer was used for detection of γ-rays. The target samples were been used 59.543 keV photons from a ^{241}Am radiative source and were detected by Si(Li) detector. Detector with a high resolution were used to count the photon intensity transistted from the compounds and the spectra were recorded. The data of this spectrum was analysed.

For each powder compound samples were sieved to 200 mesh. Sample mass thickness affect gama ray emission. Prepared by spreading powder sample compound on a mylar film at 0.0224-0.1975 g/cm^2 mass thickness, the experimental setup used in the present study is shown in figure 1.

The mass attenuation coefficient for Br compounds were calculated at 59.543 keV. The net record and count with (I) absorber and without (I_0) absorber were obtained for the same time duration and under the same experimental conditions. Incident photon unattenuation intensity and transmission photon attenuation intensity for $CaBr_2$ is shown in figure 2 & 3.

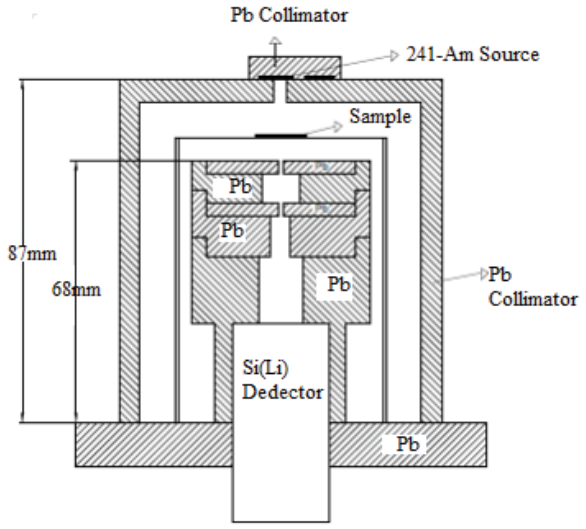

Figure 1 Schematic view of the transmision experimental geometry.

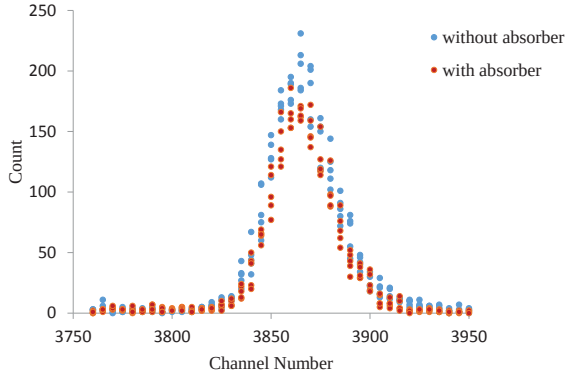

Figure 2 Unattenuation intensity and attenuation intensity for $CaBr_2$.

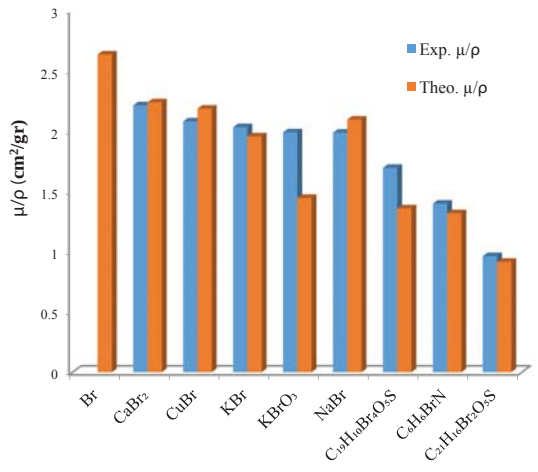

Figure 3 Comparison of experimental and theoretical values of mass attenuation coefficient μ/ρ of Br compounds.

RESULTS

The experimental and theoretical data from this study for bromine compounds have been listed in tables 1-3. The results obtained for Br compounds are pure Br for μ/ρ it ranges from 15.92% to 63.17% has been observed.

Atomic, moleculer and electronic cross sections, effective atomic number, effective electron densities and Kerma values of for some Br compounds were calculated by using mass attenuation coefficients which were obtained from experimentally. These conclusions derived from the experimental results were compared to theorically calculated values. It is concluded that the effective atomic number (Z_{eff}), effective electron density and Kerma depend on the chemical environment of a compound under investigation. When the results for Br compounds were compared with the result for pure Br, it was observed that for Kerma it ranged from 15.93% to 63.15%. The chemical environment of a compound represent a rapport between element and ligand. It is observed that the atomic weight of the element possess compound is bound to the increase of the μ/ρ values on the contrary N_{eff} values decrease. C_6H_6BrN has owned the high electron density values with $10.665x10^{+23}$. Measured values of Z_{eff} for Br (Br = 35) and compounds are given table 1. From the present results, it is found that the compound $KBrO_3$ having maximum Z_{eff} values of 39.928. Besides, it is clear that $C_{21}H_{16}Br_2O_5S$ maximum is 45.3%. The minimum KBr variation is 3.96 % in the Zeff, which may be explcined by its composition whith potassium element. Depending on the effective atomic number, the values of the electron density also depend on the atomic number of the elements that make up the compound. In general, it has been observed that the effective electron density of compounds consisting of elements with small atomic numbers has lower values. The overall error in the experimental parameters were the sum of the uncertainties in diffrent factors, as the evaluation of peak areas (2%-6%) and target mass thickness (1.45%-3.20%). Although the differences in the experimental and theoretical values observed as a result of the cross section were consistent within the error limits, some deviations were observed in some values. The reason for these deviations is assumed to be that inter molecular interactions are ignored when applying the mixing rule. Hence, these studies may help us to understand the occurrence of the absorption in compounds chemical structure and physical behavior of the compound under investigation. It is clear that all these parameters are affected with the change in chemical nature of the given elements due to its nearby lying ligands.

DISCUSSION

The present results constitute the first measurement so it was not possible to compare the findings reported in the literature. The obtained teoric results were not parallel with elements and its compounds. Additionally, experimental uncertainties can not be explained by theoretical values.

Table 1: The mass attenuation coefficient μ/ρ (cm^2/g), total moleculer cross section σ_{tm} (cm^2/molecul), total atomic cross section σ_{ta} (cm^2/atom) and effective atomic number theoretically and experimentally values for Br compounds.

Compounds	μ/ρ (cm^2/gr)		σ_{tm} (cm^2/molecul)		σ_{ta} (cm^2/atom)		Z_{eff}	
	Experimental	Theorical	Experimental	Theorical	Experimental	Theorical	Experimental	Theorical
Br		2.637						35
$CaBr_2$	2.217 ± 0.006	2.242	73.609×10^{-23}	74.440×10^{-23}	24.536×10^{-23}	24.813×10^{-23}	33.115	33.489
CuBr	2.084 ± 0.006	2.189	49.658×10^{-23}	52.160×10^{-23}	24.829×10^{-23}	26.080×10^{-23}	31.202	32.774
KBr	2.036 ± 0.005	1.960	40.246×10^{-23}	38.744×10^{-23}	20.123×10^{-23}	19.372×10^{-23}	33.612	32.357
NaBr	1.991 ± 0.013	2.099	34.030×10^{-23}	35.876×10^{-23}	17.015×10^{-23}	17.938×10^{-23}	31.528	33.238
$KBrO_3$	1.993 ± 0.005	1.452	55.287×10^{-23}	40.297×10^{-23}	11.057×10^{-23}	8.055×10^{-23}	39.928	29.089
$C_{19}H_{10}Br_4O_5S$	1.700 ± 0.007	1.365	189.182×10^{-23}	151.902×10^{-23}	4.855×10^{-23}	3.894×10^{-23}	30.979	24.852
C_6H_6BrN	1.405 ± 0.021	1.325	40.163×10^{-23}	37.860×10^{-23}	2.868×10^{-23}	2.704×10^{-23}	23.092	21.767
$C_{21}H_{16}Br_2O_5S$	0.971 ± 0.036	0.9245	87.207×10^{-23}	82.962×10^{-23}	1.937×10^{-23}	1.843×10^{-23}	19.136	18.205

Table 2: σ_{te} (cm^2/electron), N_{eff} (electron/gram) atomic parameters theoretically and experimentally values for Br compounds.

Compounds	σ_{te}		N_{eff}	
	Experimental	Theorical	Experimental	Theorical
$CaBr_2$	0.740×10^{-23}	0.740×10^{-23}	$2.992 \times 10^{+23}$	$3.025 \times 10^{+23}$
CuBr	0.795×10^{-23}	0.795×10^{-23}	$2.618 \times 10^{+23}$	$2.750 \times 10^{+23}$
KBr	0.598×10^{-23}	0.598×10^{-23}	$3.400 \times 10^{+23}$	$3.273 \times 10^{+23}$
NaBr	0.539×10^{-23}	0.539×10^{-23}	$3.689 \times 10^{+23}$	$3.889 \times 10^{+23}$
$KBrO_3$	0.276×10^{-23}	0.276×10^{-23}	$7.196 \times 10^{+23}$	$5.243 \times 10^{+23}$
$C_{19}H_{10}Br_4O_5S$	0.156×10^{-23}	0.156×10^{-23}	$10.847 \times 10^{+23}$	$8.709 \times 10^{+23}$
C_6H_6BrN	$0{,}124 \times 10^{-23}$	0.124×10^{-23}	$11.314 \times 10^{+23}$	$10.665 \times 10^{+23}$
$C_{21}H_{16}Br_2O_5S$	0.101×10^{-23}	0.101×10^{-23}	$9.596 \times 10^{+23}$	$9.129 \times 10^{+23}$

The effective electron density decreases or increases depending on the type of bonding compound molecules. It is concluded that the mass attenuation coefficient effective atomic number and electron density parameters depend on the environment of compound material. This result may be attributed to understand chemical and molecular environment of present halogen compounds. It is clear that mass attenuation coefficient and total atomic cross section depend on different interactions between central atom and ligands in the chemical compounds. This result of effective atomic number be used for compound gamma ray mass shield. These results of the present study may be used for medical applications of these compounds. The compound with a minimum Kerma value of 5.196 is $C_{21}H_{16}Br_2O_5S$ where is shown in table 3.

CONCLUSION

Atomic, moleculer and electronic cross sections, effective atomic number and electron densities, Kerma values of for some Br compounds were calculated by using mass attenuation coefficients. This study provide new insight into the literature since effective atomic number experimental values of some Br compounds have not been determined before. This research has thrown up many questions in need of further suggestion. Since Br has an unfilled 4p shell, they are sensitive to radiation interaction effects. According to the results shown in mass attenuation coefficient, Z_{eff} and N_{eff} of Br compounds are closely associated with chemical structure. Br molecules have different interatomic bond distances between ligands and central atom. As indicated the results of the present study useable for medical applications of bromine compounds. In this study, it is thought that the bromine compounds studied could be used as gamma ray shielding material due to the high values of the mass attenuation coefficient. It has also been found that the mass attenuation coefficient of some bromine compounds tends to increase with increasing Br concentration. In the light of this information fluorescence yield and jump ratio can be calculated for bromine compounds via the values in this publication. This study is a reference for future researchers due to the nature of manuscript the values obtained from the compounds studied in this values can be used as a reference in future studies. It is thought that bromine compounds can be alternative as protective material in terms of having high molecular weight. As indicated the results of the present study useable for medical applications of these compounds.

Table 3: Kerma theoretically and experimentally values for Br compounds.

Compounds	Kerma (K)	
	Experimental	Theorical
$CaBr_2$	11.855	11.989
CuBr	11.144	11.705
KBr	10.887	10.481
NaBr	10.647	11.224
$KBrO_3$	10.657	7.764
$C_{19}H_{10}Br_4O_5S$	9.091	7.299
C_6H_6BrN	7.513	7.085
$C_{21}H_{16}Br_2O_5S$	5.196	4.943

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