The Mass Attenuation Coefficients, Effective Atomic Cross Sections, Effective Atomic Numbers and Electron Densities of Some Halides

Shivalinga Gowda

Abstract—The total mass attenuation coefficients \( \mu/\rho \), of some halides such as, NaCl, KCl, CuCl, NaBr, KBr, RbCl, AgCl, NaI, KI, AgBr, CsI, HgCl\(_2\), CdI\(_2\) and HgI\(_2\) were determined at photon energies 279.2, 320.07, 514.0, 661.6, 1115.5, 1173.2 and 1332.5 keV in a well-collimated narrow beam good geometry set-up using a high resolution, hyper pure germanium detector. The mass attenuation coefficients and the effective atomic cross sections are found to be in good agreement with the XCOM values. From these mass attenuation coefficients, the effective atomic cross sections \( \sigma_a \) of the compounds were determined. These effective atomic cross section \( \sigma_a \) data so obtained are then used to compute the effective atomic numbers \( Z_{\text{eff}} \). For this, the interpolation of total attenuation cross-sections of photons of energy \( E \) in elements of atomic number \( Z \) was performed by using the logarithmic regression analysis of the data measured by the authors and reported earlier for the above said energies along with XCOM data for standard energies. The best-fit coefficients in the photon energy range of 250 to 350 keV, 350 to 500 keV, 500 to 700 keV, 700 to 1000 keV and 1000 to 1500 keV by a piecewise interpolation method were then used to find the \( Z_{\text{eff}} \) of the compounds with respect to the effective atomic cross section \( \sigma_a \) from the relation obtained by piece wise interpolation method. Using these \( Z_{\text{eff}} \) values, the electron densities \( N_\text{el} \) of halides were also determined. The present \( Z_{\text{eff}} \) and \( N_\text{el} \) values of halides are found to be in good agreement with the values calculated from XCOM data and other available published values.

Keywords—Mass attenuation coefficient, atomic cross-section, effective atomic number, electron density.

I. INTRODUCTION

The total mass attenuation coefficients or cross-sections, effective atomic numbers and electron densities are the basic quantities required in determining the penetration of X-ray and \( \gamma \)-photons in matter. With the extensive use of radio isotopes in medical, industrial and agricultural fields, the study on absorption of X-ray and \( \gamma \)-ray photons in composite materials is an interesting field of research. The knowledge of mass attenuation coefficients of X-rays and \( \gamma \)-photons in biological and other important materials is of significant interest for industrial, biological, agricultural and medical applications. Accurate values of photon mass attenuation coefficients or cross sections are needed to establish the regions of validity (keV to few MeV) of theory based parameterization, in addition to providing essential data in such diverse fields such as radiation dosimetry, radiation protection, nuclear medicine, nuclear diagnostics (computerized tomography), gamma ray fluorescence studies, and radiation biophysics. Accurate determination of the mass attenuation coefficients or cross sections in various composite materials is therefore essential in the development of high accuracy semi-empirical formulation [1]. Mass attenuation coefficients tend to increase with increasing atomic number at the same photon energy, so the materials with high atomic numbers (high mass attenuation coefficients) are normally chosen to shield X- and \( \gamma \)-radiation [2].

The scattering and absorption of X-ray and \( \gamma \)-ray radiations are related to the density and atomic number of an element. In composite materials, it is related to the density and the effective atomic number. A single number therefore cannot represent the atomic number uniquely across the entire energy region, as in the case of pure elements. This number for composite materials is called the “effective atomic number” (\( Z_{\text{eff}} \)) and varies with the energy [3]. Following Hine’s suggestions, many attempts have been made to determine the effective atomic number (\( Z_{\text{eff}} \)) for partial and total interactions in composite materials such as Alloys [4]–[9], Dosimetric compounds [10]–[14], [17]. Organic and Inorganic compounds [16], [18]–[25], Shielding materials [15]. Some empirically deduced formulae have also been reported [3], [26], [27] but their validity is limited to the experimental conditions. Tabulations of photon mass attenuation coefficients and interaction cross sections have been reported for elements and mixtures [28]. Berger and Hubbell [29] developed a computer program, XCOM, which calculates photon cross sections for partial, total interactions and attenuation coefficients for pure elements and some mixtures in the energy range of 1 keV to 100 GeV.

In this paper, we report the accurate values of total mass attenuation coefficients, effective atomic cross sections, effective atomic numbers, and the electron densities of halides at the energies 279.2, 320.07, 514.0, 661.6, 1115.5, 1173.2 and 1332.5 keV obtained by experiments. These attenuation coefficient values were used to determine the effective atomic number and hence the effective electron density of some halides as indicated earlier. We also found the elemental cross sections of the elements from the attenuation cross sections of the compounds by mixture rule [30]. The E- and Z-wise interpolation of attenuation cross sections of these elements was performed by using the logarithmic regression analysis of
the data measured by the authors and reported earlier in the 
energies of interest; 279.2, 320.07, 514.0, 661.6, 1115.5 and 
1332.5 keV along with XCOM data for standard energies 
between 250 - 1500 keV. The best-fit coefficients obtained in 
the energy range 250 – 350 keV, 350 – 500 keV, 500 – 700 
keV, 700 – 1000 keV and 1000 – 1500 keV by a piecewise 
interpolation method [17], [18] were then used to find the 
effective atomic number and electron density of halides.

II. THE METHOD OF COMPUTATION AND THEORETICAL 
Basis

Commonly employed method of obtaining effective atomic 
number Z_{eff} of a material consisting of different elements in 
definite proportions is based on the determination of total 
attenuation cross-section for photon interaction by the 
transmission method. To obtain Z_{eff} of various materials or 
compounds, the main requirements are the total mass 
attenuation coefficients, total atomic cross-sections, and 
total electronic cross-sections.

As the materials are composed of various elements, it is 
assumed that the contribution of each element of the 
compound to total photon interaction is additive, yielding the 
well-known ‘mixture rule’ [30] that represents the total mass 
attenuation coefficient (μ/ρ)_c of any compound as the sum of 
the appropriately weighted proportions of the individual 
atoms. Thus,

\[
\left( \frac{\mu}{\rho} \right)_c = \sum w_i \left( \frac{\mu}{\rho} \right)_i
\]

(1)

where, (μ/ρ)_i is the photon mass attenuation coefficient for 
the compound, (μ/ρ)_i is the photon mass attenuation coefficient 
for the individual elements in the compound, and w_i is the 
fractional weight of the elements in that compound. The mass 
attenuation cross section is proportional to the total molecular 
interaction cross section σ_i, through the relation

\[
\sigma_i = \frac{M}{N_A} \left( \frac{\mu}{\rho} \right)_c
\]

(2)

where, M = Σ_i n_i A_i is the molecular weight of the compound, 
N_A is the Avogadro’s number, and n_i is the total number of 
atoms of the constituent element, and A_i is its atomic weight.

For any compound, a quantity called the effective atomic 
cross section σ_a is defined from (2). Clearly, in calculating σ_a, 
averaging is carried out over atoms of all the elements in the 
compound. Thus, we have,

\[
\sigma_a = \frac{(\mu/\rho)_c}{N} \sum w_i A_i = \frac{1}{N} \sum A_i \left( \frac{\mu}{\rho} \right)_i = \frac{\sigma}{\Sigma_i n_i}
\]

(3)

where, \( f_i = (n_i/\Sigma n_i) \) and \( A_i \) are the fractional abundance 
and atomic weight respectively of the constituent element i. Here, 
n_i is the total number of atoms of the constituent element and 
\( \Sigma n_i \) are the total number of atoms of all types present in 
the compound as per its chemical formula, and \( \Sigma n_i \) is the total 
number of atoms in the compound. Similarly, the average 
electronic cross-section, \( \sigma_{el} \) is given by

\[
\sigma_{el} = \frac{1}{N} \sum A_i \left( \frac{\mu}{\rho} \right)_i
\]

(4)

The effective atomic number Z_{eff}, can now be written as

\[
Z_{eff} = \frac{\sigma}{\sigma_{el}}
\]

(5)

Other expressions for the effective atomic numbers are 
found in [25]-[27]. The effective electron number or electron 
density, N_{el} (number of electrons per unit mass) can be found from

\[
N_{el} = \frac{(\mu/\rho)_c}{\sigma_{el}} = \frac{A}{M} \frac{Z_{eff}}{\sum_i n_i}
\]

(6)

III. EXPERIMENTAL SET-UP AND MEASUREMENTS

In the present work the mass attenuation coefficients (μ/ρ) 
of halides were measured by transmission method employed in 
a narrow beam good geometry setup [17] using HpGe 
detector for the energies 279.2, 320.07, 514.0, 661.6, 1115.5, 
1173.2, 1332.5 keV. The mass attenuation coefficients were 
calculated for all halides using the relation

\[
\left( \frac{\mu}{\rho} \right)_c = \frac{\ln(I_0/I)}{\rho t}
\]

(7)

where, I_0 = unattenuated photon intensity, I = attenuated 
photon intensity and \( \rho t \) = mass per unit area in g/cm².

From the measured values of mass attenuation coefficients, 
the effective atomic cross section (σ_a) of halides are calculated 
using the relation

\[
\sigma_a = \frac{(\mu/\rho)_c}{A_i \sum w_i / A_i}
\]

(8)

The measured values of mass attenuation coefficients (μ/ρ) 
and the effective atomic cross sections (σ_a) obtained for all 
halides are listed in Tables I and II, respectively along with the 
XCOM values obtained at all photon energies of current interest. A good agreement was noticed among these values 
with the XCOM values of Berger and Hubbell [29] within the 
experimental uncertainties (2%).
IV. COMPUTATION OF EFFECTIVE ATOMIC NUMBER AND EFFECTIVE ELECTRON DENSITY UNITS

The effective atomic number for each sample was determined by using the effective atomic cross sections $\sigma_{e}$. In this method, the effective atomic number of the sample was simply taken to be that value of the atomic number of an element whose $\sigma_{e}$ matched with that of the sample in a given energy region. Clearly, this method requires a large pool of the elemental cross-section data over a wide range of energies.

<table>
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<tr>
<th>Halides</th>
<th>$\text{En} \rightarrow$ (keV)</th>
<th>$\mu/\rho$ (barn/cm$^2$/g)</th>
<th>$\mu/\rho$ (cm$^2$/g)</th>
<th>$\mu/\rho$ (barn/cm$^2$/g)</th>
<th>$\mu/\rho$ (cm$^2$/g)</th>
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<th>$\mu/\rho$ (cm$^2$/g)</th>
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Table I: Total Mass Attenuation Coefficients $\mu/\rho$ (barn/cm$^2$/g) of Halides

For this purpose, we are generating the elemental cross sections for the elements from $Z = 3$ to $Z = 70$ of all standard energies between 250 – 1500 keV from XCOM [29] along with the measured experimental cross sections in the energies 279.2, 320.0, 514.0, 661.6, 1115.5, 1173.2 and 1332.5 keV and reported earlier by using a mixture rule from the attenuation cross sections of the compounds. The elemental cross sections show a non-linear variation with respect to photon energy $E$ and atomic number $Z$. Therefore, we can assume that the relation for $\sigma$ could be of the type

$$\sigma = A(Z)E^B(Z)$$  \hspace{1cm} (9)

where, $A(Z)$ and $B(Z)$ are constants with respect to energy and vary with atomic number.

Table II: Total Mass Attenuation Coefficients $\sigma_{e}(\text{barn/atom})$ of Halides

Table III: Best-Fit Coefficients for Halides

$$\ln\sigma = \ln A(Z) + B(Z)\ln E$$  \hspace{1cm} (10)

and it represents a straight line with slope $B(Z)$ and intercept $\ln A(Z)$. For the presentation of results, the photon energy region of

International Scholarly and Scientific Research & Innovation 10(8) 2016

ISNI:0000000091950263
interest was divided into five suitable regions viz., a) 250-350 keV, b) 350-500 keV, c) 500-700 keV, d) 700-1000 keV and e) 1000-1500 keV. Within each of these regions, the values of \( \ln r \) were found to vary linearly with \( \ln E \). So, a logarithmic regression analysis was performed between \( \ln r \) and \( \ln E \) in all the three energy regions and the best-fit values of the slope \( B(Z) \) and the intercept \( \ln A(Z) \) were determined. Further, we assume that the values of \( \ln A(Z) \) and \( B(Z) \) are simple functions of atomic number and are given by the relations

\[
\ln A(Z) = \ln A_1 + B_1 \ln Z \\
(11)
\]

and

\[
B(Z) = \ln A_2 + B_2 \ln Z \\
(12)
\]

### TABLE IV

<table>
<thead>
<tr>
<th>Halides</th>
<th>En ( \rightarrow ) (keV)</th>
<th>( Z_{\text{eff}} )</th>
<th>( Z_{\text{at}} )</th>
<th>( Z_{\text{at}} )</th>
<th>( Z_{\text{at}} )</th>
<th>( Z_{\text{at}} )</th>
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### TABLE V

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<td>HgCl(_2)</td>
<td>4.113</td>
<td>3.914</td>
</tr>
<tr>
<td>Cd(_2)</td>
<td>2.589</td>
<td>2.515</td>
</tr>
<tr>
<td>Hg(_2)</td>
<td>2.688</td>
<td>2.593</td>
</tr>
</tbody>
</table>

Equations (11) and (12) represent straight lines with slopes \( B_1 \) and \( B_2 \) and corresponding intercepts \( \ln A_1 \) and \( \ln A_2 \), respectively in a selected region of elements. In each energy region, the range of elements is divided into three groups. This ensures the linearity in the selected region so that the best-fit values of \( \ln A_1 \), \( B_1 \), \( \ln A_2 \) and \( B_2 \) could be obtained for the \( E \) and \( Z \) region of interest. These values are shown in Table III. Using these best - fit values further, we obtained the formula for \( Z_{\text{eff}} \) of the form

\[
Z_{\text{eff}} = \frac{\sigma}{\alpha} \left[ \frac{A}{E} \right]^{1/d} \\
(13)
\]

where, \( d = B_1 + B_2 \) \( \ln E \) and \( E \) is in keV.

In obtaining this formula, we have assumed the equivalence between \( Z_{\text{eff}} \) of the sample and the \( Z \) of the equivalent element as discussed earlier [17], [18].

Using the calculated \( Z_{\text{eff}} \) values, the effective electron density \( N_{e2} \) was calculated by using the following relation

\[
N_{e2} = \frac{N}{Z_{\text{eff}}} = \frac{N}{Z_{\text{eff}}} \sum_i n_i \\
(14)
\]
Fig. 1 Plot of $Z_{et}$ as a function of Photon Energy in keV
Fig. 2 Plot of $N_{el}$ as a function of Photon Energy in keV
The values of $Z_{\text{eff}}$ and $N_{\text{el}}$ obtained using (13) and (14) are listed in Tables IV and V, respectively. These values are compared with the values calculated in an empirical formula by using XCOM values of attenuation cross sections and the other experimental values available [20]. Plots of the present values and other available measured values of $Z_{\text{eff}}$ [20] versus energy are shown in Fig. 1, and $N_{\text{el}}$ versus energy are also shown in Fig. 2 along with the values calculated using XCOM data [29] for standard energies from $10^5$ to $10^6$ keV for all halides.

V. RESULTS AND DISCUSSION

The measured values of mass attenuation coefficients ($\mu/\rho$) and effective atomic cross sections ($\sigma_{\text{e}}$) are in good agreement with XCOM values within 2% error, whereas effective atomic numbers ($Z_{\text{eff}}$) and electron densities ($N_{\text{el}}$) are in good agreement with XCOM values within 4% error for all halides. It is observed that the variation of $Z_{\text{eff}}$ with energy depends on (spread) the difference between the atomic numbers of the constituent elements present in the compound. The materials, which have least spread in the atomic numbers of the constituents like NaCl, KCl, CsI and CdI$_2$ have almost constant values of $Z_{\text{eff}}$ and $N_{\text{el}}$. In case of CuCl, NaBr, KBr, RbCl, AgCl, NaI, AgBr, and HgI$_2$ the spread of the constituent elements is less in the compounds, hence the variation of $Z_{\text{eff}}$ and $N_{\text{el}}$ with the energy is less. Whereas, in case of KI and HgCl$_2$ there is a large spread in the atomic number of the constituents hence, there is large variation of $Z_{\text{eff}}$ and $N_{\text{el}}$ values with energy.

The variation $Z_{\text{eff}}$ and $N_{\text{el}}$ with energy are shown in Fig. 1 and 2, respectively along with the measured values of available data [20]. A typical plot of $N_{\text{el}}$ vs $Z_{\text{eff}}$ shown in Fig. 3 for all energies show a linear relationship for all compounds.

VI. CONCLUSIONS

The effective atomic number and the electron density of halides are useful parameters in radiation detectors, dosimetric calculation of radiation dose in radiotherapy and radiation shielding. These have physical meaning and their numerical values allow many characteristics of a material to be visualized, which are used as radiation detectors in biological dosimetry of ionizing radiations. They are also useful in the field of radiation monitoring, radiographic measurements.
ACKNOWLEDGEMENT

The author is grateful to Professor Ramakrishna Gowda, Department of Studies in Physics, University of Mysore, Mysore, for providing the required facilities to carrying out this work. He also expresses his gratitude to the Principal and Management of PES College of Engineering, Mandya for their support and financial assistant.

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International Scholarly and Scientific Research & Innovation 10(8) 2016 399

ISNI:0000000091950263