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MASS ATTENUATION COEFFICIENTS OF BIOLOGIAL MATERIALS USING XCOM

By

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Table of Contents

Table of Contents iv

List of Figures v

List of Tables vi

Abbreviation vi

Abstract viii

Acknowledgements ix

1. Introduction 1

- **1.1 Background of the Study** 1
  - **1.1.1 Basics of Photon Interactions with Matter** 2
  - **1.1.2 Brief Review of Related/Previous Work** 3
- **1.2 Significance of the Study** 4
- **1.3 Objectives of the Study** 5
  - **1.3.1 General objective of the study** 5
  - **1.3.2 Specific objective of the study** 5

2. Review of Literature 6

- **2.1 Interaction of gamma radiation with matter** 6
  - **2.1.1 Compton scattering** 6
  - **2.1.2 Photoelectric effect** 7
  - **2.1.3 Electron-positron pair production** 7
- **2.2 The attenuation coefficient** 8

3. Methodology 14

- **3.1 Calculation of the total mass attenuation coefficients (χ):** 14
- **3.2 Compounds under Study** 15

4. Result and Discussion 19

5. Summary and Conclusion 27

References 28

List of Figures

Figure 2 1: The relative importance of various processes of gamma radiation interaction with matter (from [1]) 11

Figure 2 2: Dependence of radiation intensity (a) and its logarithm (b) on absorber thickness........ 12

Figure 2 3: Dependence of the "partial" attenuation coefficients of lead on photon energy (a) and Dependence of the total attenuation coefficient of lead and iron on photon energy (b) 13

Figure 4. 1: Mass attenuation coefficient (cm^2/g) versus concentration (g/cm^3) of the experimental data (a) compared with XCOM-computed (b) for 81 (Black), 356 (Blue), 511 (Green), 662 (Yellow), 1173 (Orange), and 1332 (Red) photon energies (keV). 21

Figure 4. 2: XCOM computed and Experimental data of $\chi(cm^2/g)$ for each samples at 81 (Black), 356 (Blue), 511 (Green), 662 (Yellow), 1173 (Orange), and 1332 (Red) photon energies in keV at the concentration of the solution (a) 0.05, (b) 0.15 and (c) 0.25 (g/cm^3). 23

Figure 4. 3: Comparison of $\chi(cm^2/g)$ computed by XCOM with respect to experiment according to relative deviation, for (a) Glucose, (b) Maltose and (c) Sucrose, as a function of photon energies. (The concentration of each sample was 0.15 g/cm^3).......... 25

List of Tables

Table 3 1: The description of physical properties of the three common carbohydrates.................... 17

Table 3 2: The chemical formulae of saccharides and the weight fractions of hydrogen (H), carbon (C) and oxygen (O) for each. 17

Table 4. 1: Mass attenuation coefficients χ $(cm2/g)$ of solution of some carbohydrates. 20

Table 4. 2: Experimental and XCOM computed mass attenuation coefficients of solution of some carbohydrates for a given concentration. 22

Table 4. 3: Absolute percentage difference of mass attenuation coefficients χ(cm^2/g) of three different carbohydrate samples at six distinct photon energies. 24

Abbreviation

eV - - - - - - - - - - - - - electron volt

KeV - - - - - - - - - - - - - Kilo electron volt

MeV - - - - - - - - - - - - - Mega electron volt

GeV - - - - - - - - - - - - - Giga electron volt

MAC - - - - - - - - - - - - - Mass Attenuation Coefficient

Abstract

The total mass attenuation coefficients of three different carbohydrates such as glucose$(C_6H_{12}O_6)$*, maltose*$(C_{12}H_{22}O_{11})$ *and sucrose* $(C_{12}H_{22}O_{11}H_2O)$ *were determined theoretically at different photon energies using XCOM computer program(version 3.1) in the energy range of 5 keV-1.5 MeV. Specifically, the mass attenuation coefficients obtained theoretically (XCOM computed coefficients) were compared with experimental results for 81, 356, 511, 662, 1173 and 1332 keV photon energies. The XCOM computed coefficients were compared to the experimental values, the agreement between the two is within less than 2%. That is; the XCOM program is successful in the calculation of photon mass attenuation coefficients of composite materials as others found in literature.*

Key words: *mass attenuation coefficients, composite materials, photon energy*.

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Chapter One

1. Introduction

1.1 Background of the Study

The study of the interaction of gamma radiations with matter yields useful information for designing experimental arrangements for handling the isotopes decaying by gamma emission. The most important quantity characterizing the penetration and diffusion of gamma radiation in a material is the attenuation coefficient. An attenuation coefficient is a measure of the reduction in the gamma ray intensity at a particular energy caused by an absorber and the absorption coefficient is related to the amount of energy retained by the absorber as the gamma radiation passes through it. Mass attenuation coefficient is the measure of the average number of interactions between incident photons and matter that occur in a given mass per unit area of thickness of the material encountered.

Accurate values of these coefficients are necessary to establish the regions of validity of theory based parameterization in addition to providing essential data in diverse fields such as tomography, x-ray fluorescence studies and radiation biophysics. If the constants like attenuation coefficients, absorption coefficients, effective atomic numbers etc. are known, the energy absorbed in a medium can be calculated.

Atomic number for photon interaction probably cannot be represented by a single number for the *composite materials* as well as mixtures across the energy spectrum. So, we will have to have a new quantity effective atomic number for these materials and mixtures. The concept of the Z-dependence of photon interaction has many applications in radiation studies. The effective atomic number has proved to be a convenient parameter for interpreting the attenuation of *x*- or gamma rays. This has been used where radiation shields are required to protect people against nuclear particles and electromagnetic radiations by calculating the energy absorbed in a medium. The cross-sections of mixtures and composite materials can however be discussed in terms of atomic numbers. By knowing the values of effective atomic numbers, the cross-sections can be determined for a known photon energy of a radioactive source which is to be used in industries etc.

The concept of nuclear cross-section is a very convenient way to express the probability of interaction of gamma rays with target nucleus and it varies with the nature of the process involved and energy of the incident radiation. The cross-section measures the relative probability for the process to occur when a single nucleus is exposed to a beam of photons of total flux one particle per unit area. It is measured in barns (1 barn=10^{-28}m^2).

In scattering experiments, the term electron density is quite significant as it represents the number of electrons per unit volume, so the number of electrons scattered can be calculated by this quantity.

1.1.1 Basics of Photon Interactions with Matter

Interaction of photons with matter by which individual photons are removed or deflected from a primary beam of $x-$ or $\gamma-$ radiation, may be classified according to; (i) the kind of target, e.g. electrons, atoms or nuclei with which the photon interacts and (ii) the type of event, e.g. scattering, absorption, pair-production etc. which takes place.

The four types of interactions that taking place with *atomic electrons* are:

i) Photoelectric effect (Absorption)
ii) Coherent (Rayleigh)scattering (Scattering)
iii) Compton scattering (Scattering)
iv) Two photon Compton scattering (Multi photon effect)

The three types of interactions which occur with *nucleons* are:

i) Photonuclear reactions (γ, n), (γ, p), photo-fission etc. (Absorption).
ii) Elastic nuclear scattering (γ, γ) (Scattering) Iii)
iii) Inelastic nuclear scattering $(\gamma, \gamma^{/})$ (Scattering)

There are also three types of interactions with *electric field* surrounding charged particle:

i) Electron-positron pair production in the field of nucleus (Absorption)
ii) Electron-positron pair production in electron field (Absorption)
iii) Nucleon-anti-nucleon pair production (Absorption)

The two types of interactions occurring with mesons are:

i) Photo-meson production (Absorption)
ii) Modified (γ, γ) (Scattering)

Nevertheless, among all of these interaction processes, the five main processes includes:

i) Photoelectric absorbtion
ii) Compton scattering
iii) Pair production
iv) Coherent scattering
v) Photo-nuclear interactions

where the first three are the most important, as they result in the transfer of energy to electrons, which then impart that energy to matter in many coulomb-force interactions along their tracks. Rayleigh scattering is elastic, the photon is merely redirected through a small angle without any loss of energy. Photonuclear interactions are only significant for photon energies above a few MeV. The individual interaction processes are discussed In chapter 2. .

1.1.2 Brief Review of Related/Previous Work

A gamma ray is removed from a beam entirely by either absorption or scattering. The gamma rays that pass straight through, therefore, are those that have not suffered any interactions at all. They therefore retain their original energy. The total number of gamma rays is, however, reduced by the numbers that have interacted. The attenuation suffered by a gamma-ray beam can be shown, in fact, to be exponential with respect to thickness, see Eq. (2.1), i.e.

$$I(x) = I_0 e^{-\mu x}$$

where I_0 is the incident beam intensity or gamma-ray numbers, x is the thickness of absorber, μ is linear attenuation coefficient, $I(x)$ is the intensity transmitting through x thickness. The attenuation coefficient is a quantity that is characteristic of the absorbing material [1].

To understand the particle interaction in matter and its kinematics, Monte Carlo (MC) simulation tools are used [2,3]. In many scientific, engineering, and medical applications, data on the scattering and absorption of photons (X-rays, gamma-rays, bremsstrahlung) are necessary. Using a personal computer, it is possible to find cross sections and attenuation coefficients for compounds and mixtures for desired energies from 1 keV up to 100 GeV. For this purpose, the XCOM computer program is used [4].

Linear attenuation coefficient (μ) varies with the density of the absorber, even though the absorber material is the same. Therefore, the mass attenuation coefficient (χ) is much more widely used and is defined as

$$\chi = {}^{\mu}/_{\rho}$$

where ρ is the density of the medium [5].

Various studies were carried out about the calculation of the photon mass attenuation coefficients through theoretical and experimental methods in the 2000s. Some examples in relation with the subject are summarized as follows: Shirmardi et al. investigated gamma-ray mass attenuation coefficients of various barites, concretes, and lead at 0.662, 1.173, and 1.332 MeV energies using MCNP-4C code [6]. The photon mass attenuation coefficients of different absorber materials for 59.4, 661.6, and 1332.5 keV energies were determined experimentally by Abdel-Rahman et al. [7]. El-Sersy et al. studied the gamma-ray mass attenuation coefficients of various glass systems [8]. Photon mass attenuation values of different gemstones were calculated by Medhat [9]. Medhat also calculated the photon mass attenuation coefficients for different types of composite materials by means of theoretical and experimental methods and he also compared the obtained coefficient values with XCOM results[10]. Mass attenuation coefficients of gold, bronze, and water at different impurities were calculated by MCNP-4C code and also compared to XCOM values by Esfandiari et al. [11]. Medhat and Wang carried out a study about mass attenuation coefficients of various scintillator materials such as BaF2 , BGO, and NaI(Tl) and compared them with the XCOM results [12].

1.2 Significance of the Study

In this work, the photon mass attenuation coefficients of Glucose, Maltose and Sucrose composite materials are calculated using the XCOM programs at different photon energy ranges. In addition, calculated mass attenuation coefficients by choosing various photon energies are also compared with each other and the literature values. It is found that the calculated mass attenuation coefficients are very close to the literature values.

1.3 Objectives of the Study

1.3.1 General objective of the study

The general purpose of this work will be to investigate the mass attenuation coefficients for some different mono and disaccharides for photon energies in the range of 5 keV–1.5 MeV.

1.3.2 Specific objective of the study

The Specific objectives of this work are:

- To calculate the mass attenuation coefficients of Glucose, Maltose and Sucrose theoretically for photon energies in the range of 5 keV–1.5 MeV.
- To compare the mass attenuation coefficients obtained theoretically with experimental results for the corresponding photon energies 81, 356, 511, 662, 1173 and 1332 keV.

Chapter Two

2. Review of Literature

2.1 Interaction of gamma radiation with matter

As in the case of charged particles (e. g., electrons, protons, alpha particles), interaction of photons of gamma radiation with matter is of electromagnetic nature. However, the exact physical mechanism of that interaction is quite different than in the case of charged particles, because:

- Photons do not have electric charge, therefore they do not participate in Coulomb interaction. Photon interaction cross-section is much smaller than interaction cross-sections of charged particles.
- The photon rest mass is zero, therefore their velocity is always equal to the velocity of light. I. e., photons cannot be slowed down in matter (unlike charged particles). Photons can be only scattered or absorbed.

Photon absorption is an interaction process when the photon disappears and all its energy is transferred to atoms of the material or to secondary particles. Photon scattering is an interaction process when the photon does not disappear, but changes direction of its propagation. In addition, the scattered photon may transfer a part of its energy to an atom or an electron of the material. There are two interaction processes whereby a photon is absorbed and several types of scattering (of which one type is much more important than the others). Those interaction processes are defined below.

2.1.1 Compton scattering

From the quantum mechanical point of view, a scattering event is a collision of two particles a photon and an electron or a photon and an atom. From the laws of conservation of energy and momentum it follows that due to scattering by electrons of the material photon energy must decrease (because a part of that energy must be transferred to the electrons). This effect, which was first described in 1922 by

American physicist A. Compton, became one of the cornerstones of quantum mechanics, because it proved that electromagnetic radiation under certain circumstances behaves like particles. Such type of scattering, when photon energy decreases, is called Compton scattering. When photon energy is large (of the order of 10 keV or more), Compton scattering is the dominant scattering mechanism. Since a single Compton scattering event is a result of photon's interaction with a single electron, the *atomic* Compton scattering cross-section σ_C is equal to the *electronic* Compton scattering crosssection σ_{Ce} times the number of electrons in an atom (the latter number is equal to the atomic number Z):

$$\sigma_C = Z\sigma_{Ce} \tag{2.1.1}$$

By definition, σ_{Ce} does not depend on Z. Thus, the atomic Compton scattering cross-section is directly proportional to the atomic number of the material. When the photon energy is sufficiently large (of the order of 100 keV or larger), σ_{Ce} decreases with increasing photon energy.

2.1.2 Photoelectric effect

Photoelectric effect is a type of interaction of a photon with an atom when the atom absorbs all energy of the photon (i. e. the photon disappears) and one of atomic electrons is removed from the atom.

That electron is called the photoelectron. The atomic cross-section of the photoelectric effect is characterized by an especially strong dependence on the atomic number Z of the material and on photon energy. When photon energy is of the order of 100 keV, the just-mentioned cross-section is approximately equal to

$$\sigma_f = \frac{10^{-37}Z^5}{(hv)^{7/2}} \tag{2.1.2}$$

where the cross-section σ_f is expressed in m^2, and hv is the photon energy in MeV. From Eq. (2.1.2) it follows that photoelectric effect cross-section rapidly increases with increasing atomic number Z and decreasing photon energy hv.

2.1.3 Electron-positron pair production

In the electric field of an atomic nucleus, a photon may stop existing by transforming all its energy into relativistic energy of two new particles – *a* free electron and a positron (electron’s antiparticle). Since the recoil energy of the nucleus is relatively small, the law of conservation of energy during such an event can be written as follows:

$$hv = m_+c^2 + m_-c^2 \tag{2.1.3}$$

where m_+c^2 and m_-c^2 are the total relativistic energies of the positron and the electron (m_+ and m_- are the total relativistic masses of the positron and the electron). Since m_+ and m_- are always larger than the electron’s rest mass m0, from (2.1.3) it follows that pair production is only possible when photon energy is larger than two rest energies of an electron: $2m_0c^2 \approx 1.02$ MeV. This is the so-called “threshold energy” of pair production. Although pair production becomes possible when photon energy exceeds the mentioned threshold value, the pair production cross-section σ_p exceeds the Compton scattering cross-section σ_C only when the photon energy approaches and exceeds 10 MeV. At photon energies less than 3 MeV, the frequency of pair production events is much smaller than the frequency of Compton scattering events.

2.2 The attenuation coefficient

The physics upon which this technique is based depends on the fact that the gamma-ray attenuation is a function of both the photon energy and the elemental composition of the material. When a well-collimated narrow beam of photons passes through a homogeneous sample of thickness x, the ratio of the transmitted beam intensity I, emerging from the target along the incident beam direction, to the incident beam intensity I_0 is given by Lambert's law,

$$\frac{I(x)}{I_0} = e^{-\mu x} \tag{2.1}$$

This equation assumes that no scattered photons reach the detector, and μ is the linear attenuation coefficient of the element μ(μ has unit of cm^{-1}). The linear attenuation coefficient is related to the mean-free-path τ by the expression

$$\mu = \frac{1}{\tau} \tag{2.2}$$

The mean free path of a photon, of a given energy traveling in an element, is the average distance that the photon can travel without interacting with the element. The mass attenuation is an alternate expression for the attenuation coefficient of an element. The mass attenuation coefficient χ (χ has unit of cm^2/g), involving the density ρ, is given by the expression,

$$\chi = \frac{\mu}{\rho} \tag{2.3}$$

Note that unit of the *linear* attenuation coefficient μ is measured in cm^{-1} or /cm while the unit of the *mass* attenuation coefficient χ is cm^2/g:

$$[\chi] = \frac{[\mu]}{[\rho]} = \frac{cm^{-1}}{g/cm^3} = cm^2/g$$

When the material consists of a chemical compound or of a *homogeneous* mechanical mixture such as a composite, the linear attenuation coefficient is given by the weighted sum of the linear coefficients of the components. This is known as the rule-of-mixture.

Thus,

$$\mu = \sum_{i}^{k} \mu_i w_i \tag{2.4a}$$

and

$$\sum_{j=1}^{k} w_j = 1 \tag{2.4b}$$

where $\mu_i$is the linear attenuation of the *i-th* element and w_i is its proportion by weight. For a chemical compound with the chemical formula $(Z_1)_{a1}(Z_2)_{a2}(Z_3)_{a3}\ldots(Z_n)_{an}$ where Z_i's are the atomic number of the elements, the weighting factor for the *i-th* element, Z_i, is given by

$$w_i = \frac{\mathrm{a_i A_i}}{\sum_{j=1}^{n} \mathrm{a_j A_j}} \tag{2.5}$$

where $\mathrm{A_j}$'s are the atomic weight of the element, and $\mathrm{a_j}$'s are the number of atoms of the element in the chemical formula [10].

By using Lambert's law and the rule-of-mixtures, we can obtain sufficient information to determine the constituent materials of the composite by measuring the attenuation of the initial gamma-ray beam at a number of selected energies as the beam passes through the composite. Therefore, the x-ray attenuation in materials can be expressed in the following general form using Lambert's law and the rule-of-mixtures,

$$\frac{I(E_j)}{I_0(E_j)} = \exp\left[-\sum(\mu_i(E_j)x_i)\right] \tag{2.6}$$

where *i* denotes the components in the composite, and j denotes the energies at which the parameters are measured. $I_0(E_j)$ is the incident beam intensity, $I(E_j)$ is the transmitted beam intensity, x_i is the thickness of component *i*, and $\mu_i(E_j)$) is the linear attenuation coefficient of component *i* measured at E_j.

In order to study a two component composite a minimum of two energies are required. This gives us the following two equations,

$$\xi(E_1) = \mu_1(E_1)x_1 + \mu_2(E_1)x_2 \tag{2.7a}$$

and

$$\xi(E_2) = \mu_1(E_2)x_1 + \mu_2(E_2)x_2 \tag{2.7b}$$

where

$$\xi(E_j) = -\ln\left[\frac{I(E_j)}{I_0(E_j)}\right] \equiv \ln\left[\frac{I_0(E_j)}{I(E_j)}\right] \tag{2.8}$$

The linear attenuation coefficients for elements, or compounds, can be either obtained from experimental measurements or can be obtained from XCOM predictions [4]. Then, by taking the attenuation measurements of the initial beam at carefully chosen energies, it is sufficient information to solve the two simultaneous Eqs. (2.7a) and (2.7b) which proved us:

$$x_1 = \frac{\xi(E_1)\mu_2(E_2) - \xi(E_2)\mu_2(E_1)`}{\mu_1(E_1)\mu_2(E_2) - \mu_1(E_2)\mu_2(E_1)} \tag{2.9a}$$

and

$$x_2 = \frac{\xi(E_2)\mu_1(E_1) - \xi(E_1)\mu_1(E_2)`}{\mu_1(E_1)\mu_2(E_2) - \mu_1(E_2)\mu_2(E_1)} \tag{2.9b}$$

Though the work presented here studies two component composites, this does not exclude the capability of this x-ray technique for studying composites with more than two components. To study such composites, one needs to measure the attenuation of the beam at more energies along the x-ray spectrum according to the number of components.

In making these measurements one has the choice of energies to use. There are many constraints such as x-ray penetration through material, measurement time and maximum energy of the x-ray source that may influence the energy selections. Thus within these constraints, one wishes to optimize the accuracy of the thickness determination. In next section the derived expressions for quantitatively assessing the accuracy of the technique outlined above for a two component composite are presented based on Ref. [14].

The total cross-section of interaction

The total cross-section of interaction of a gamma radiation photon with an atom is equal to the sum of all three mentioned partial cross-sections:

$$\sigma = \sigma_C + \sigma_f + \sigma_P \tag{2.10}$$

Depending on the photon energy and the absorber material, one of the three partial cross-sections may become much larger than the other two. Then the corresponding interaction process is the dominant one. Fig. 2.1 shows the intervals of photon energy $h\nu$ and atomic number Z corresponding to the case when one of the three interaction processes dominates.

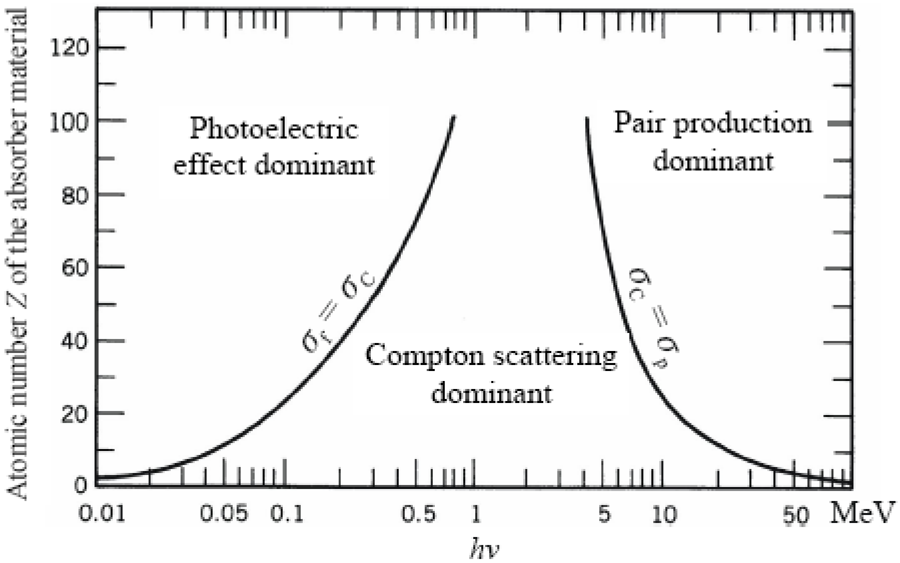


Figure 2 *1: The relative importance of various processes of gamma radiation interaction with matter (from [1])*

Obviously, the photoelectric effect dominates at small values of photon energy, Compton scattering dominates at intermediate energies, and pair production dominates at high energies. The width of the energy interval corresponding to the Compton effect increases with decreasing atomic number of the material.

Using the definition of interaction cross-section, it is easy to derive the dependence of gamma radiation intensity on thickness of absorber material. If a narrow parallel beam of gamma radiation falls normally to a layer of absorber material, and if the detector only detects the photons that passed through that layer without any kind of interaction with its material, then the dependence of detected radiation intensity I on the layer thickness x is exponential:

$$I(x) = I_0 e^{-\sigma n_a x} \tag{2.11}$$

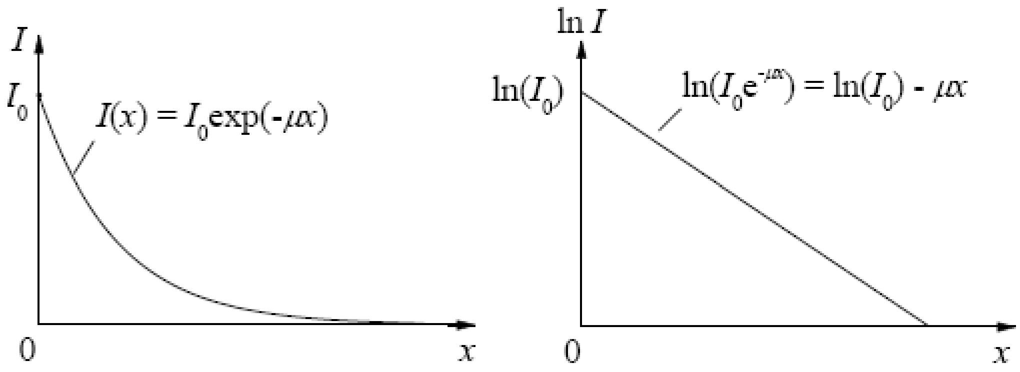
where I_0 is the intensity of the incident beam, and n_a is the atomic concentration in the material. This Eq. (2.11) is equal to Eq. (2.1) and it can be written as:

$$I(x) = I_0 e^{-\mu x} \tag{2.12}$$

since the attenuation coefficient μ is:

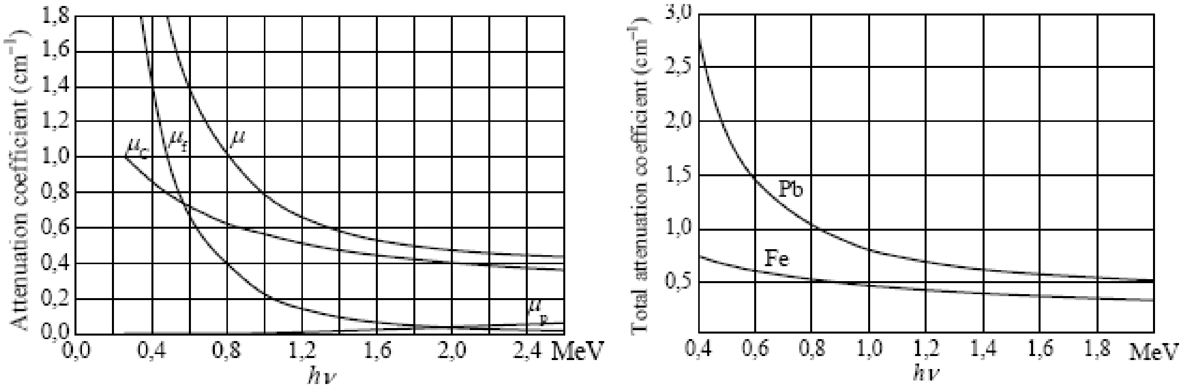
$$\mu = \sigma n_a \tag{2.13}$$

The exponential function (2.12) is shown graphically in Figure 2.2 Fig.ure 2.2b suggest the method of measuring the attenuation coefficient μ: it is obtained by linear fitting of the dependence of intensity logarithm on absorber thickness.



(a) (b)

Figure 2 2: Dependence of radiation intensity (a) and its logarithm (b) on absorber thickness



(a) (b)

Figure 2 3: Dependence of the “partial” attenuation coefficients of lead on photon energy (a) and Dependence of the total attenuation coefficient of lead and iron on photon energy (b)

Since the interaction cross-section is a sum of cross-sections of three types of interaction (see (2.10)), the attenuation coefficient μ can be expressed as a sum of three “partial” attenuation coefficients corresponding to each of the three interaction processes:

$$\mu = \mu_C + \mu_f + \mu_P \qquad (2.11)$$

Expressions of the coefficients μ_C, μ_f and μ_P are obtained by substituting the σ in (2.13) by a corresponding partial cross-section. When characterizing an absorber material, it is sometimes more convenient to use the so-called “mass attenuation coefficient” instead of the attenuation coefficient defined above. The mass attenuation coefficient is defined as the ratio of the attenuation coefficient and absorber density (see Eq.(2.3)).

If Compton scattering is the dominant interaction process, then different absorbers are characterized by approximately equal mass attenuation coefficients. This is because the atomic cross section of Compton scattering is proportional to the atomic number Z (see (2.1.1)). Then the attenuation coefficient (2.3) is proportional to the electron concentration Zn_a, which, in turn, is proportional to density ρ of the material. If the attenuation coefficient is strongly influenced by other interaction processes (photoelectric effect and pair production), then the expression of the attenuation coefficient includes the terms proportional to higher powers of the atomic number Z (the photoelectric cross-section is proportional to Z^5 and the pair production cross-section is proportional to Z^2). In this case, the attenuation coefficient μ is no longer proportional to ρ (in other words, the mass attenuation coefficient is no longer constant).

Chapter Three

3. Methodology

Photon attenuation coefficients or cross sections are of great significance in both fundamental and applied science. They are invaluable in many applied fields, such as nuclear diagnostics, radiation protection, nuclear medicine, radiation dosimetry etc. In medical and biological applications the photon energy range of general interest is from 5 keV to a few MeV. Nevertheless, the amount of γ-ray attenuation data for many compounds, for example biological samples, is limited (Nair et al., 1993; Hubbell, 1994; Chitralekha et al., 2005). Recent reviews (Hubbell, 1999; Cesareo, 1999; Hubbell, 2000) emphasize the need for further attenuation measurements on biological samples.

3.1 Calculation of the total mass attenuation coefficients (χ):

In shielding calculations, materials made of homogeneous mixture of elements are frequently encountered. For a mixture of known composition, the total mass attenuation coefficient can be determined from basic data by relationships [1]. That is, the mass attenuation coefficient, $\chi = \mu/\rho$ ($\mathrm{cm^2/g}$), for any chemical compound or mixture is given by additively rule

$$\chi = \sum_{i}^{k} w_i \left(\frac{\mu}{\rho}\right)_{\mathrm{i}} \tag{3.1}$$

where w_i and (μ/ρ)i are the weight fraction and the mass attenuation coefficient, respectively, of the ith element. In a compound, the weight fraction of the ith element is given by

$$w_i = \frac{\mathrm{a_i A_i}}{\sum_{j=1}^{n} \mathrm{a_j A_j}} \tag{3.2}$$

where $\mathrm{A_j}$'s are the atomic weight of the element, and $\mathrm{a_j}$'s are the number of atoms of the element in the chemical formula.

The total linear attenuation coefficients (μ) were calculated for the 3 (solution of carbohydrates) composite samples using a computer program called XCOM (version 3.1). The used XCOM program and database cross sections for elements ranging from Z=1 to 100 have been recently modified to calculate the total mass attenuation coefficients (χ) for elements, compounds and mixtures from 1keV upto 100 GeV [4], and provides total cross section as well as partial cross sections for various interaction processes. With a known density (ρ) of shield materials, the total linear attenuation coefficients (μ) were extracted from calculated results of XCOM.

The density of composite materials was calculated using the rule of mixtures formula given by the following equation [16]:

$$\rho_c = V_f \rho_f + \left(1 - V_f\right)\rho_m \tag{3.3}$$

where ρ_c, ρ_f and ρ_m are density of composite, reinforcement and the matrix materials respectively while V_f is the fractional volume for reinforcement material. V_f could be calculated from the equation:

$$V_f = \frac{1}{\left(1 + \left(\frac{1-w}{w}\right)\frac{\rho_f}{\rho_m}\right)} \tag{3.4}$$

where w is fractional weight for reinforcement materials. It is calculated by

$$w = \frac{W_f}{W_c} \times 100\% = \frac{W_f}{W_f + W_m} \times 100\% \tag{3.5}$$

where W_c, W_f and W_m are weight of composite, reinforcement and matrix materials respectively [17].

3.2 Compounds under Study

The main goal of this study is focused on testing the applicability of XCOM database for studying mass attenuations coefficients for a sample of composite materials for photon energy range 5-1.5 keV photon energies. The XCOM computed results of mass attenuation coefficients were compared with the experimental data, obtained from Ref. [18], for the same samples and a good agreement has been observed. The modeling for photon interaction parameters was standard for any type of composite samples. Specifically, this work would compute the mass attenuation coefficients of Carbohydrates (mono and disaccharides).

Carbohydrates are an important class of naturally occurring substances found in both plant and animal matter:

- Glucose, the most abundant carbohydrate, has the chemical formula

$$\mathrm{C_6H_{12}O_6} \quad \text{or} \quad \mathrm{C_6(H_2}O)_6.$$

- Fructose and manose are isomers having the same chemical composition. Glucose, fructose and manose are examples of monosaccharides, simple sugars that cannot be broken into smaller molecules by hydrolysis with aqueous acids. Two monosaccharide units can be linked together to form a disaccharide. Sucrose, lactose and maltose are three common disaccharides.
- The chemical formula of Maltose is

$$C_{12}H_{22}O_{11}H_2O$$

- The chemical formula of Sucrose is

$$C_{12}H_{22}O_{11}$$

Calculations of the photon mass attenuation coefficients of the investigated composite materials would be carried out by the XCOM theoretically. It can generate cross-sections and attenuation coefficients for elements, compounds or mixtures in the energy ranges between 1kev-100 GeV, in the form of total cross-sections and attenuation coefficients as well as partial cross-sections of the following processes: incoherent scattering, coherent scattering, photoelectric absorption and pair production in the field of the atomic nucleus and in the field of the atomic electrons [10]. However, this work was concerned with the calculations of the total mass attenuation coefficients of carbohydrates sample at 81, 356, 511, 662, 1173 and 1332 keV photon energies.

The choice of the studied composite materials hinges on their multifaceted importance. Carbohydrates are very important in chemical, biological, nutritional and medical fields and are extensively used in the food, textile, oil drilling and thermal as well as nuclear power industries. They perform a variety of physiological functions in living organisms. Carbohydrates in the form of sugar and starch represent a major part of the total caloric intake by humans, by most animal life and by microorganisms. They play a vital role in all living cells. The description of compounds chosen (carbohydrates) is given below:

Table 3 1: The description of physical properties of the three common carbohydrates

Physical Properties	**Glucose** $C_6H_{12}O_6$	**Maltose** $C_{12}H_{22}O_{11}H_2O$	**Sucrose** $C_{12}H_{22}O_{11}$
Grade	Lab. Reagent	Lab. Reagent	Lab. Reagent
Trade mark	Qualigens	Qualigens	Qualigens
Molecular weight (g)	180.16	360.32	342.3
Density (g/cm^3)	1.562	1.54	1.58
Melting point	146℃	102-103℃	185-186℃
Boiling point	110℃	112℃	110℃
Solubility in 100 parts	60	50	60

We generated the mass attenuation coefficients for these Carbohydrates from XCOM using the chemical compositions given by International Encyclopedia of Composites [4]. The chemical formula of the saccharides and the weight fractions of hydrogen, carbon and oxygen in them are given in Table 3.2.

Table 3 2: The chemical formulae of saccharides and the weight fractions of hydrogen (H), carbon (C) and oxygen (O) for each.

Saccharides		**Chemical Formula**	**Weight Fractions of**		
			H	C	O
Monosaccharide:	Glucose,	$C_6H_{12}O_6$	0.0672	0.4	0.5328
Disaccharide:	Maltose	$C_{12}H_{22}O_{11}$	0.0648	0.4211	0.5141
	Sucrose,	$C_{12}H_{22}O_{11}H_2O$	0.0648	0.4211	0.5141

Methods

$C_6H_{12}O_6$, $C_{12}H_{22}O_{11}H_2O$ and $C_{12}H_{22}O_{11}$ solutions were used for the determination of the photon mass attenuation coefficients. The concentration of our sample with corresponding density of the solution (see table 3.3) were performed based on Eq. (3.3), (3.4) and (3.5).

Table 3. 3 Density of the solution for a given concentration.

Sample		Concentration (g/cm^3)				
		0.05	0.10	0.15	0.20	0.25
Density of the solution (g/cm^3)	Glucose	1.015360	1.032520	1.048891	1.067814	1.079843
	Maltose	1.014850	1.031378	1.047539	1.064687	1.082157
	Sucrose	1.016029	1.033682	1.051168	1.069724	1.079751

The result obtained at six different photon energies; 81, 356, 511, 662, 1173 and 1332 keV would be recorded or tabulated and analyzed. In addition, these materials were chosen so that they were the same as those in the literature and it was possible to compare directly the results from experiment [18].

Chapter Four

4. Result and Discussion

The mass attenuation coefficients of the samples were determined using XCOM (version 3.1) method. The XCOM computer program able to compute the mass attenuation coefficients of elements, compounds and others for photon energy ranges from 1 keV – 100 GeV. For the purpose of our work we computed the mass attenuation coefficients for three carbohydrate samples namely, Glucose, Maltose and Sucrose (the description of the physical properties of our samples has been already presented in Table 3.1) for photon energy ranges from 5keV – 1.5 MeV.

In particular, the mass attenuation coefficients of solution of some three carbohydrates of experimental data and the theoretical values obtained using XCOM database for five different concentrations (g/cm^3), (0.05, 0.10, 0.15, 0.20 and 0.25), each at six different photon energies, (81, 356, 511, 662, 1173 and 1332 keV) were recorded in Tables 4.1. The source of experimental data was Gagagndeep Sandhu, PHD Dissertation, Amritsar India, 2001.

Table 4.1 together with Figure 4.1 discusses that photon mass attenuation coefficient computed using XCOM DATABASE is almost the same as the experimental data found in literature [18], for all the three sample (Glucose, Maltose and Sucrose). As we see from Figure 4.1, the mass attenuation coefficient (both computed−"a" and experiment−"b") decreases as increasing photon energy for each five concentration, 0.05, 0.10, 0.15, 0.20 and 0.025 g/cm^3.

It is clear that there is satisfactory agreement between experiment and theory, although the experimental values tend to be lower than the theory, as more detail has been discussed using Table 4.3 and Figure 4.3. According to Ref. [10], discrepancy in the values of the calculated and the experimental mass attenuation coefficients could be due to deviations from narrow-beam geometry in the source–detector arrangements.

Table 4. 1: Mass attenuation coefficients χ (cm^2/g) of solution of some carbohydrates.

Sample	Density of the solution g/cm^3)	Conc. (g/cm^3)		Mass attenuation coefficients χ(cm^2/g)					
				81 keV	**356 keV**	**511 keV**	**662 keV**	**1173 keV**	**1332 keV**
Glucose $(C_6H_{12}O_6)$	1.015360	0.05	*a*	0.1819	0.1107	0.0952	0.0852	0.0651	0.0606
			b	0.1824	0.1109	0.0958	0.0855	0.0652	0.0611
	1.032520	0.10	*a*	0.1813	0.1105	0.0949	0.0851	0.0648	0.0600
			b	0.1820	0.1107	0.0956	0.0854	0.0651	0.0610
	1.048891	0.15	*a*	0.1808	0.1104	0.0946	0.0849	0.0646	0.0597
			b	0.1816	0.1105	0.0954	0.0852	0.0650	0.0609
	1.067814	0.20	*a*	0.1805	0.1102	0.0944	0.0848	0.0654	0.0594
			b	0.1813	0.1103	0.0953	0.0851	0.0649	0.0608
	1.079843	0.25	*a*	0.1800	0.1100	0.0939	0.0847	0.0638	0.0592
			b	0.1810	0.1101	0.0952	0.085	0.0648	0.0607
Maltose $C_{12}H_{22}O_{11}H_2O$	1.014850	0.05	*a*	0.1822	0.1104	0.0954	0.0852	0.0648	0.0609
			b	0.1823	0.1108	0.0957	0.0855	0.0651	0.0615
	1.031378	0.10	*a*	0.1813	0.1103	0.0950	0.0851	0.0644	0.0607
			b	0.1819	0.1106	0.0955	0.0854	0.0650	0.0612
	1.047539	0.15	*a*	0.1808	0.1102	0.0946	0.0849	0.0643	0.0606
			b	0.1814	0.1104	0.0953	0.0852	0.0649	0.0610
	1.064687	0.20	*a*	0.1806	0.1100	0.0939	0.0848	0.0642	0.0603
			b	0.1801	0.1102	0.0952	0.0851	0.0648	0.0609
	1.082157	0.25	*a*	0.1801	0.1098	0.0937	0.0847	0.0640	0.0600
			b	0.1809	0.1100	0.0951	0.085	0.0647	0.0605
Sucrose $C_{12}H_{22}O_{11}$	1.016029	0.05	*a*	0.1821	0.1105	0.0952	0.0851	0.0651	0.0608
			b	0.1824	0.1100	0.0957	0.0856	0.0651	0.0610
	1.033682	0.10	*a*	0.1811	0.1103	0.0949	0.085	0.0647	0.0605
			b	0.1820	0.1107	0.0956	0.0854	0.0650	0.0609
	1.051168	0.15	*a*	0.1806	0.1098	0.0942	0.0849	0.0641	0.0603
			b	0.1816	0.1105	0.0955	0.0853	0.0649	0.0608
	1.069724	0.20	*a*	0.1804	0.1096	0.0937	0.0848	0.0639	0.0600
			b	0.1811	0.1103	0.0953	0.0851	0.0648	0.0607
	1.079751	0.25	*a*	0.1802	0.1094	0.0934	0.0847	0.0636	0.0599
			b	0.1810	0.1810	0.0951	0.0850	0.0647	0.0606

(The symbol a and b refers to "Experiment" and "XCOM Computed", respectively)

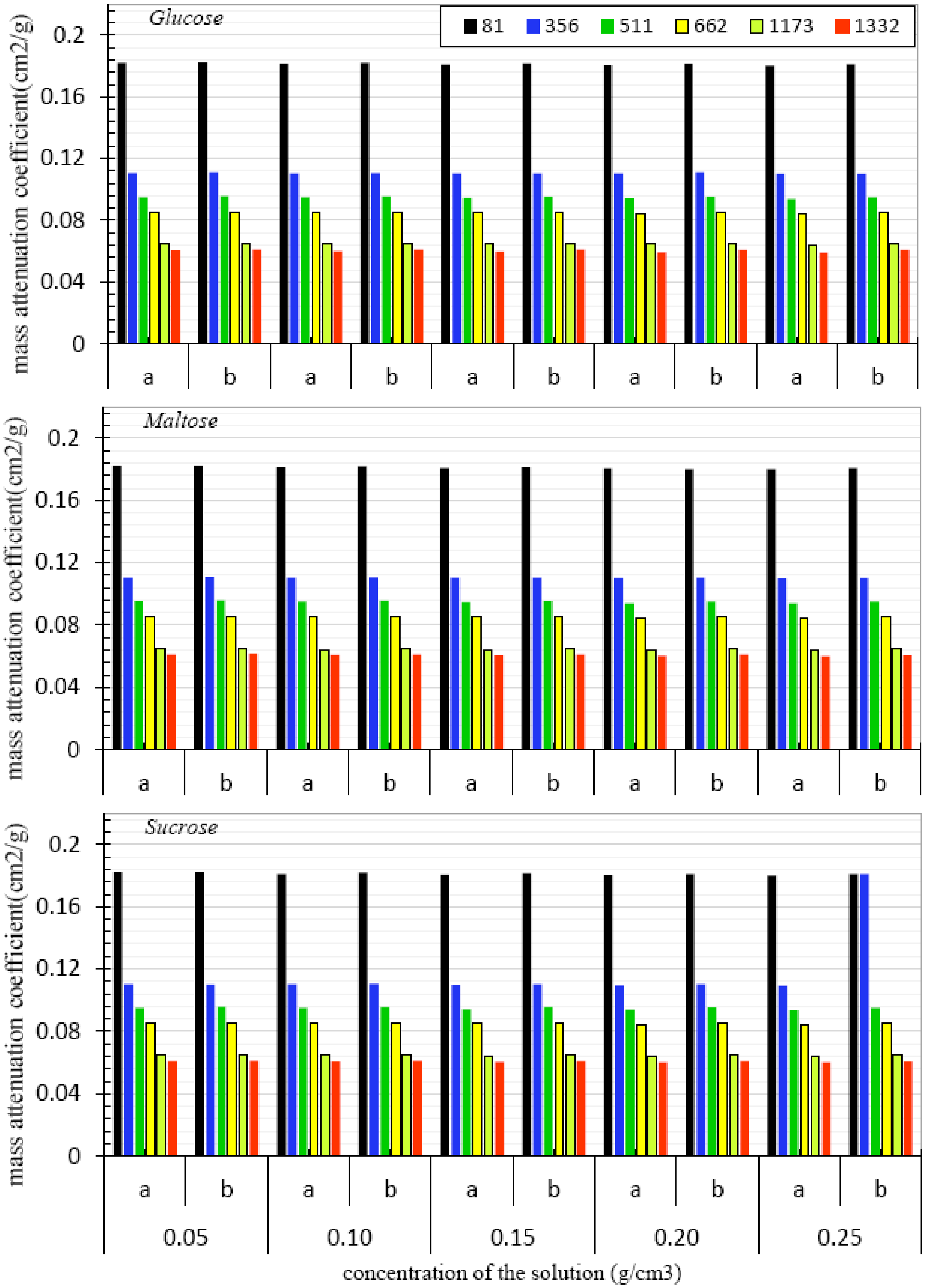


Figure 4. 1: Mass attenuation coefficient (cm^2/g) versus concentration (g/cm^3) of the experimental data (a) compared with XCOM-computed (b) for 81 (Black), 356 (Blue), 511 (Green), 662 (Yellow), 1173 (Orange), and 1332 (Red) photon energies (keV).

Furthermore, the results of experimental data were compared with the theoretical values obtained using XCOM database of the three carbohydrates solution for concentrations (g/cm^3) of 0.05, 0.15 and 0.25 each at six different photon energies: 81, 356, 511, 662, 1173 and 1332 keV (see Tables 4.2).

Table 4. 2: Experimental and XCOM computed mass attenuation coefficients of solution of some carbohydrates for a given concentration.

Conc. (g/cm^3)	**Photon Energy (keV)**	**Mass Attenuation Coefficients** χ in cm^2/g					
		Glucose		**Maltose**		**Sucrose**	
		Experiment	**Computed**	**Experiment**	**Computed**	**Experiment**	**Computed**
0.05	81	0.1808	0.1816	0.1808	0.1814	0.1806	0.1816
	356	0.1104	0.1105	0.1102	0.1104	0.1098	0.1105
	511	0.0946	0.0954	0.0946	0.0953	0.0942	0.0955
	662	0.0849	0.0852	0.0849	0.0852	0.0849	0.0853
	1173	0.0649	0.0650	0.0643	0.0649	0.0641	0.0649
	1332	0.0597	0.0609	0.0606	0.0610	0.0603	0.0608
0.15	81	0.1808	0.1816	0.1808	0.1814	0.1806	0.1816
	356	0.1104	0.1105	0.1102	0.1104	0.1098	0.1105
	511	0.0946	0.0954	0.0946	0.0953	0.0942	0.0955
	662	0.0849	0.0852	0.0849	0.0852	0.0849	0.0853
	1173	0.0649	0.065	0.0643	0.0649	0.0641	0.0649
	1332	0.0597	0.0609	0.0606	0.061	0.0603	0.0608
0.25	81	0.18	0.181	0.1801	0.1809	0.1802	0.181
	356	0.11	0.1101	0.1098	0.11	0.1094	0.181
	511	0.0939	0.0952	0.0937	0.0951	0.0934	0.0951
	662	0.0847	0.085	0.0847	0.085	0.0847	0.085
	1173	0.0638	0.0648	0.064	0.0647	0.0636	0.0647
	1332	0.0592	0.0607	0.06	0.0605	0.0599	0.0606

Source of experimental data: Gagagndeep Sandhu, PHD Dissertation, Amritsar India, 2001

More clearly, Figure 4.2 discusses that the mass attenuation coefficients decreases with increasing photon energy for each of the three samples (Glucose, Maltose and Sucrose) for the three concentrations (a) 0.05, (b) 0.15, and (c) 0.25 in g/cm^3.

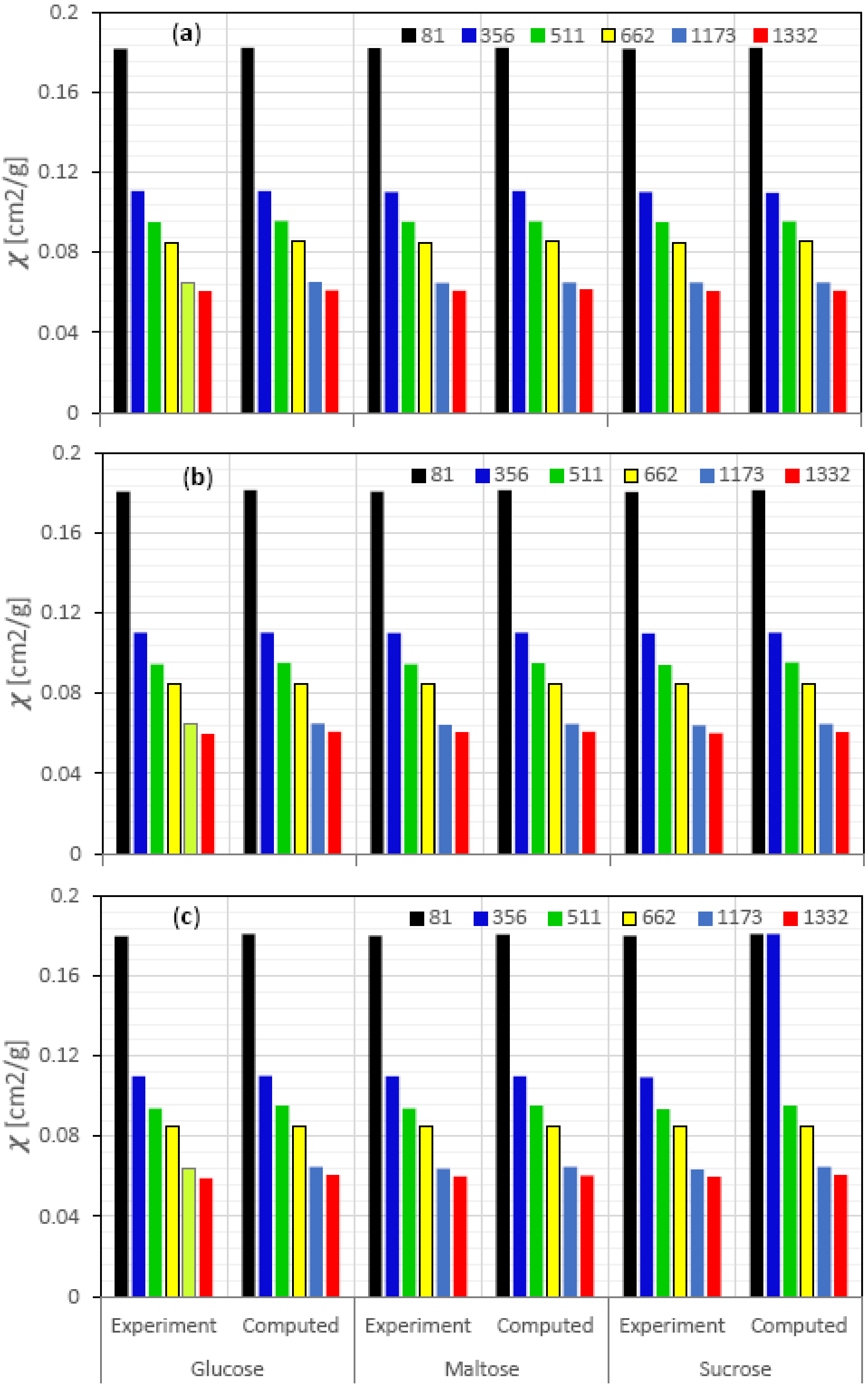


Figure 4. 2: XCOM computed and Experimental data of $\chi(cm^2/g)$ for each samples at 81 (Black), 356 (Blue), 511 (Green), 662 (Yellow), 1173 (Orange), and 1332 (Red) photon energies in keV at the concentration of the solution (a) 0.05, (b) 0.15 and (c) 0.25 (g/cm^3).

The relative percentage difference (PD%) between the mass attenuation coefficients of the samples (conc. 0.15 g/cm^3) were evaluated between XCOM computed and experimental data. The results are presented in Table 4.3. For each samples, the results found below 2% for all six discrete photon energies in our consideration. Therefore, the use of carbohydrates based composite materials may be considered as a substitute material for Glucose, Maltose and Sucrose for radiotherapy and nuclear medicine uses.

Table 4. 3: Absolute percentage difference of mass attenuation coefficients χ(cm^2/g) of three different carbohydrate samples at six distinct photon energies.

Sample (Conc. 0.15 g/cm^3)	**Energy (keV)**	$\chi\ (cm^2/g)$		**Difference**	$\boldsymbol{PD}^*$
		a	b	$a - b$	**(%)**
Glucose $C_6H_{12}O_6$	81	0.1808	0.1816	-0.0008	**0.4**
	356	0.1104	0.1105	-0.0001	**0.1**
	511	0.0946	0.0954	-0.0008	**0.8**
	662	0.0849	0.0852	-0.0003	**0.4**
	1173	0.0649	0.0650	-0.0001	**0.6**
	1332	0.0597	0.0609	-0.0012	**2.0**
Maltose $C_{12}H_{22}O_{11}H_2O$	81	0.1808	0.1814	-0.0006	**0.3**
	356	0.1102	0.1104	-0.0002	**0.2**
	511	0.0946	0.0953	-0.0007	**0.7**
	662	0.0849	0.0852	-0.0003	**0.4**
	1173	0.0643	0.0649	-0.0006	**0.9**
	1332	0.0606	0.0610	-0.0004	**0.7**
Sucrose $C_{12}H_{22}O_{11}$	81	0.1806	0.1816	-0.0010	**0.6**
	356	0.1098	0.1105	-0.0007	**0.6**
	511	0.0942	0.0955	-0.0013	**1.4**
	662	0.0849	0.0853	-0.0004	**0.5**
	1173	0.0641	0.0649	-0.0008	**1.2**
	1332	0.0603	0.0608	-0.0005	**0.8**

*PD stands for Percentage Difference

The percentage difference (PD) was calculated by

$$\boldsymbol{PD}(\%) = \frac{a - b}{a} \times 100\%$$

where a and b represent experimental and XCOM Computed, respectively.

It is clear that there is a good agreement between experiment and XCOM computed, although the experimental values tend to be slightly greater than the XCOM computed.

According to Table 4.3 the percentage difference of mass attenuation coefficients reads a minimum of 0.1% and a maximum of 2.0%, that is; the error (*PD*%) of XCOM is found below 2%. In addition, Figure 4.3 also discusses the good agreements between experiment and XCOM computed based on the data recorded in Table 4.3.

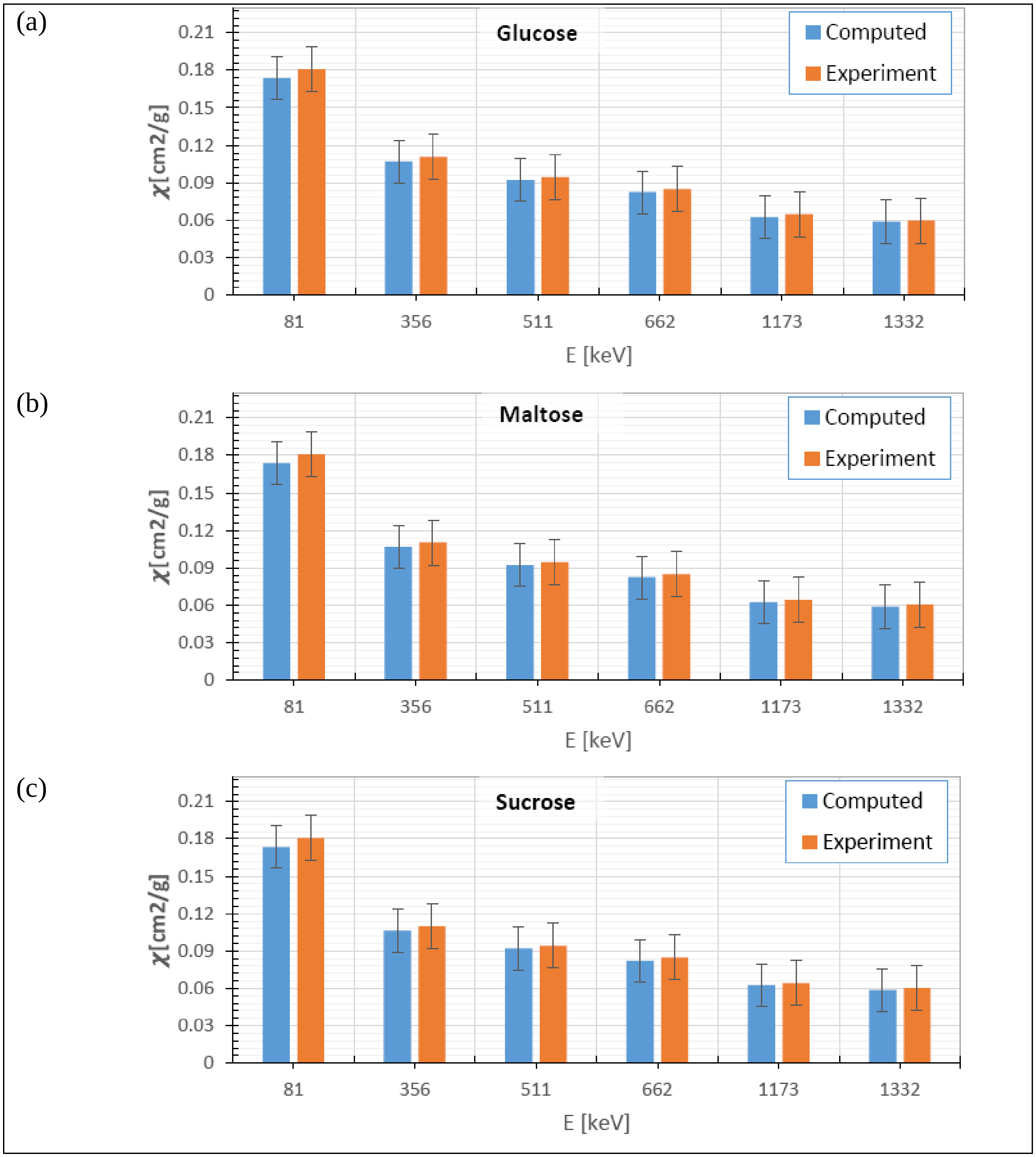


Figure 4. 3: Comparison of $\chi(cm^2/g)$ computed by XCOM with respect to experiment according to relative deviation, for (a) Glucose, (b) Maltose and (c) Sucrose, as a function of photon energies. (The concentration of each sample was 0.15 g/cm^3)

Therefore, the percent deviation of the experimental values from the XCOM computed values is between 0.1% and 2.0% as shown in Table 4.3 (and Figure 4.3). Since the XCOM computations are expected to yield values with an error of 2% (Hubbell, 1999), it may safely assumed that the experimental set up used in the study was adequate to measure χ with accuracy comparable to that of theory.

Chapter Five

5. Summary and Conclusion

In order to derive values for the mass attenuation coefficient from the measured incident and transmitted gamma ray intensities, it is necessary to know the thickness and bulk density of each sample of the system. Calculations of the mass attenuation coefficients of the investigated composite materials were carried out by the XCOM theoretically. It can generate cross-sections and attenuation coefficients for elements, compounds or mixtures in the energy range between 1 keV and 100 GeV, in the form of total cross-sections and attenuation coefficients as well as partial cross-sections of the following processes: incoherent scattering, coherent scattering, photoelectric absorption and pair production in the field of the atomic nucleus and in the field of the atomic electrons.

The relative deviations between the experimental and theoretical values are lower than the corresponding values of XCOM for most common carbohydrates at different photon energies as shown in Figures 4.1, 4.2 and 4.3. It is clear that the representative experimental measured data for mass attenuation coefficients of all the samples are a function of incident photon energy and the chemical compositions. The mass attenuation coefficients of the selected composite samples are different based on the chemical compositions of the elements.

In this work we used the XCOM program (version3.1) to calculate the mass attenuation coefficients of three different carbohydrates such as glucose($C_6H_{12}O_6$), maltose($C_{12}H_{22}O_{11}$) and sucrose ($C_{12}H_{22}O_{11}H_2O$) in the 5keV up to 1.5 MeV photon energy range. The results of the mass attenuation coefficients at 81, 356, 511, 662, 1173 and 1332 keV photon energies of the samples were determined and tabulated. The XCOM computed coefficients were compared with experimental results. The agreement between the two is within less than 2%. That is, the result show that the XCOM computed mass attenuation values are close to experimental values. These results conclude that XCOM database can be applied to estimate the fundamental parameter mass attenuation coefficients for various attenuator and energies. Therefore, we can conclude that the XCOM database is useful theoretical method for evaluation of photon interaction parameters of the various types of composite materials.

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Declaration

I declare that the project work here by submitted to Addis Ababa University for the degree of Master of science in Physics has not been previously submitted by me for a degree at this or any other university, and it is my own work both in design and execution, and that all material contained herein has been duly acknowledged.

Name: ______Sahile Derese_______

Signature: ____________________

This MSc. project has been submitted to for examination with my approval as University advisor.

Name: ____________________________ (PhD)

Signature:____________________________

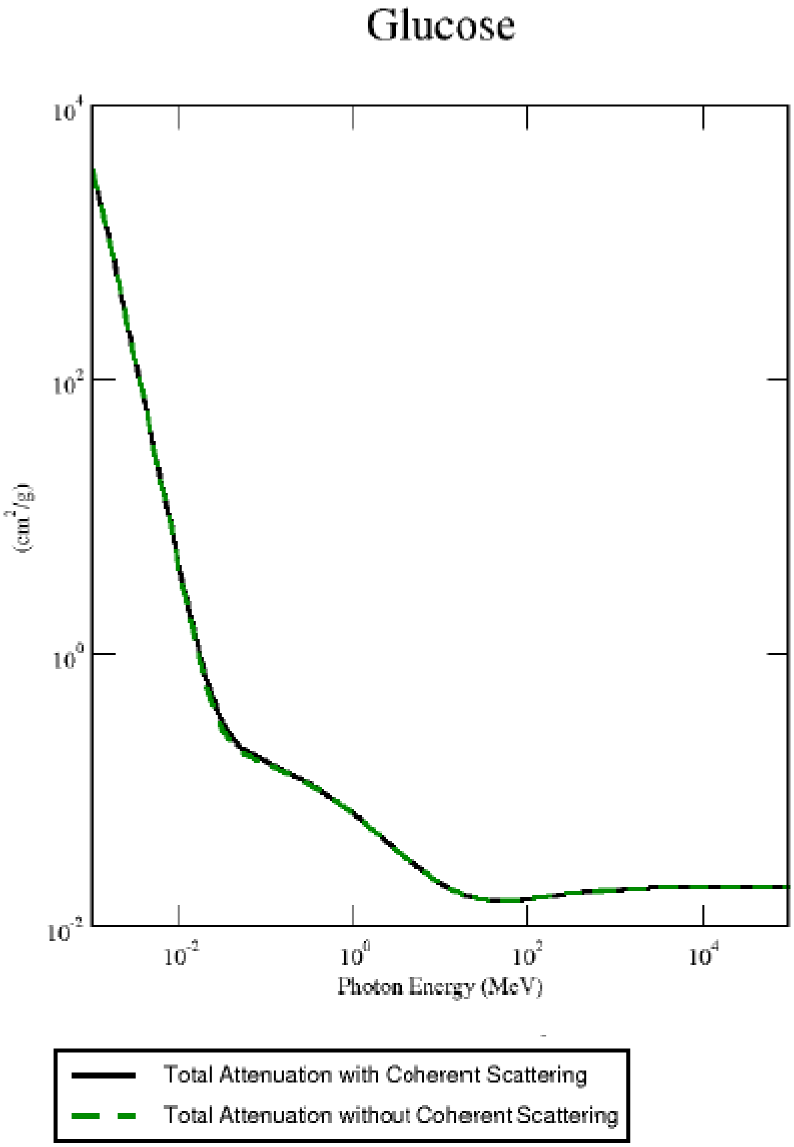
Place and Date of Submission: Addis Ababa University

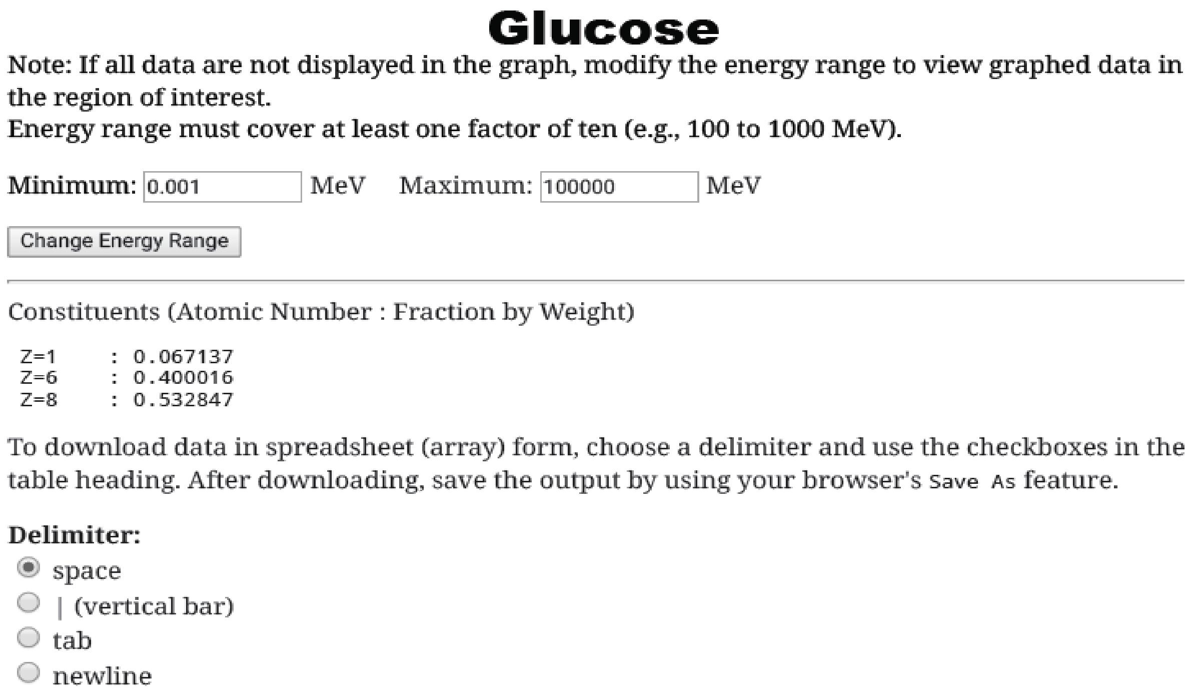
Department of Physics

November, 2021

Appendix: Sample XCOM output

XCOM





Glucose

Note: If all data are not displayed in the graph, modify the energy range to view graphed data in the region of interest.
Energy range must cover at least one factor of ten (e.g., 100 to 1000 MeV).

Minimum: 0.001 MeV Maximum: 100000 MeV

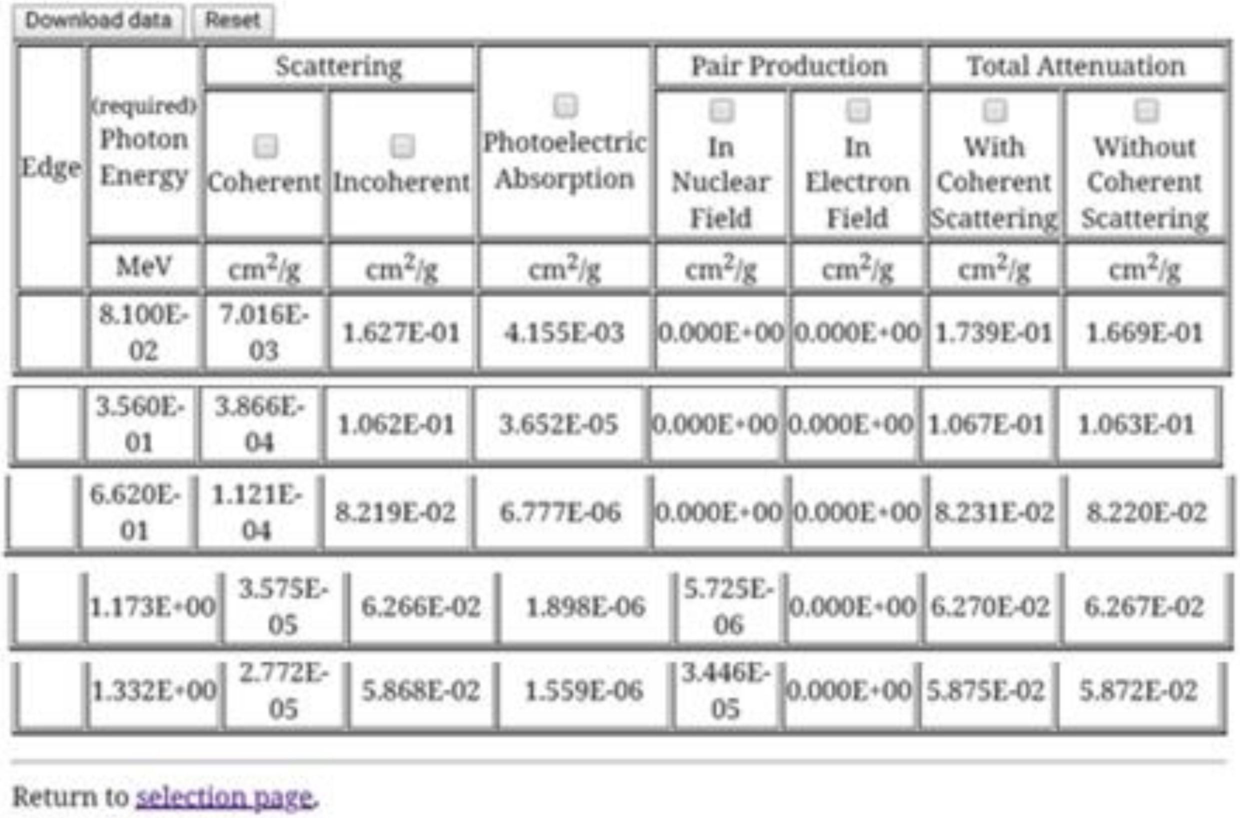
Constituents (Atomic Number : Fraction by Weight)

```
Z=1     : 0.067137
Z=6     : 0.400016
Z=8     : 0.532847
```

To download data in spreadsheet (array) form, choose a delimiter and use the checkboxes in the table heading. After downloading, save the output by using your browser's `Save As` feature.

Delimiter:

● space
○ | (vertical bar)
○ tab
○ newline



Edge	(required) Photon Energy	Scattering		☐ Photoelectric Absorption	Pair Production		Total Attenuation	
		☐ Coherent	☐ Incoherent		☐ In Nuclear Field	☐ In Electron Field	☐ With Coherent Scattering	☐ Without Coherent Scattering
	MeV	cm²/g	cm²/g	cm²/g	cm²/g	cm²/g	cm²/g	cm²/g
	8.100E-02	7.016E-03	1.627E-01	4.155E-03	0.000E+00	0.000E+00	1.739E-01	1.669E-01
	3.560E-01	3.866E-04	1.062E-01	3.652E-05	0.000E+00	0.000E+00	1.067E-01	1.063E-01
	6.620E-01	1.121E-04	8.219E-02	6.777E-06	0.000E+00	0.000E+00	8.231E-02	8.220E-02
	1.173E+00	3.575E-05	6.266E-02	1.898E-06	5.725E-06	0.000E+00	6.270E-02	6.267E-02
	1.332E+00	2.772E-05	5.868E-02	1.559E-06	3.446E-05	0.000E+00	5.875E-02	5.872E-02

Return to selection page.