Kirkuk University Journal /Scientific Studies (KUJSS)
Volume 10, Issue 3, September 2015 , p.p(92-107)
ISSN 1992 - 0849

Study of γ-ray energy losses in the ionic crystals using Monte Carlo code

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Received date: 30 / 11 / 2014 **Accepted date: 8 / 3 / 2015**

ABSTRACT

In this paper, measurements were carried out of the calculated attenuation of the ranges gamma rays energy(279,356,479,662) KeV and using radioactive sources (Hg^{203}, Ba^{133}, W^{189}, Cs^{137}). In the current results has determined (μ_L, μ_m) by using Monte Carlo simulation (i.e. through the account of each of the intensity falling and intensity transmit in samples proposed in search) .permission has been drawing relationship graphs between the logarithm of the absorbance and thickness proposed for each of the ionic crystals (CsI, CdTe), hence slope graphs relationship represents attenuation coefficient linear and thereafter are calculated attenuation coefficient mass through during the relationship the following ($\mu_m = \mu_L / \rho$), and the results showed the current search using the Monte Carlo that the values of coefficients mass attenuation of gamma rays in crystals (CsI, CdTe) converge and overlap with each other at high energies the fact that the attenuation depends vitally on Compton scattering , either the values of attenuation coefficients linear showed a variation the obvious fact that the attenuation coefficient depends on the density of the absorbed . Addition, the study was examine to calculate the total atomic cross section and electron density, and the results of this study showed good agreement with the XCOM package.

Keywords: *Monte Carlo simulation, XCOM package,γ_Rays, Ionic Crystals.*

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Volume 10, Issue 3, September 2015 , p.p(92-107)
ISSN 1992 - 0849

دراسة فقدان طاقة اشعة كاما في البلورات الايونية باستخدام برنامج مونت كارلو

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تاريخ استلام البحث: 30 / 11 / 2014 تاريخ قبول البحث: 8 /3/ 2015

الملخص

اجريت حسابات نظرية لدراسة التوهين اشعة كاما لمديات الطاقة (279,356,479,662)KeV وباستخدام المصادر المشعة (Hg^{203},Ba^{133},W^{189},Cs^{137}) وفي النتائج الحالية تمت قياس (μ_L, μ_m) بواسطة برنامج مونت كارلو (اي من خلال حساب كل من الشدة الساقطة والشدة النافذة من النماذج المقترحة في البحث) اذن تم رسم العلاقة البيانية بين لوغاريتم الامتصاصية والسمك المقترح لكل من البلورات الايونية (CsI,CdTe), اذ ان ميل العلاقة البيانية يمثل معامل التوهين الخطي وبعد ذلك يتم حساب معامل التوهين الكتلي من خلال خلال العلاقة الاتية ($\mu_m = \mu_L/\rho$), كما اظهرت النتائج البحث الحالي باستخدام برنامج مونت كارلو ان قيم معاملات التوهين الكتلي لأشعة كاما في البلورات(CsI,CdTe) تتقارب وتتداخل مع بعضها عند الطاقات العالية كون التوهين يعتمد بدرجة اساسية على تاثير كومبتن ،اما قيم معاملات التوهين الخطي فقد اظهرت تباينا واضحاً كون معامل التوهين يعتمد على كثافة الممتصة. اضافة الى ذلك تم حساب مساحة المقطع العرضي والكثافة الكترونية للبلورات الايونية، واظهرت نتائج البحث الحالي توافقاً جيداً مع النتائج برنامج (XCOM).

الكلمات الدالة :محاكاة مونت كارلو،XCOM package ،أشعة كاما، البلورات الايونية.

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1.INTRODUCTION

Ionic Crystals are a class of crystals in which the lattice –site occupants are charged ions ,.They are perhaps the simplest type of chemical bonding to visualize since it is almost totally electrostatic in nature [1].The criterion for such bonding is the difference in electro negativity, and as such occurs between electropositive elements and electro negativity elements (generally electropositive elements from group I or II and electro negativity elements from group VI or VII [2].The mass attenuation and energy absorption coefficient are broad used in the study of interaction of gamma rays with matter .There are three interactions occurs between the photons and the atoms apart from other types over a wide range of energies .By irradiating the material with $\gamma - Rays$,ionization of the material takes place and the stored energy of the material increases[3].There have been a great number of experimental and theoretical investigations to determine mass attenuation coefficient values in various elements and compound – mixtures. Hubbel reported (μ_m) values for 40 elements and 45 mixtures and compounds over the energy from (1KeV-20MeV)[4].Gamma –ray attenuation coefficients have been determined experimentally using a narrow beam transmission method for PbO-SiO_2 glasses system at 662,1173 and 1332 KeV photon energies[5].Determine the mass attenuation coefficient for members of BaO-B_2O_3 glass system at various energies in the 356-1332 KeV range[6].The mass attenuation coefficient is a fundamental factor to derive interaction parameters of diametric and shielding interest such as molecular ,atomic and electronic cross sections ,effective atomic number ,electron density ,energy deposition and shielding effectiveness[7-9].The photon interaction with matter is combination of partial interactions namely photoelectric absorption ,Compton scattering and pair production .The mass attenuation coefficients of individual elements are being employed XCOM program in energy (1KeV-100GeV)[10].Scattering and absorption of $\gamma - Rays$ is related to the density and atomic numbers of an elements. In composite materials, it is related to the effective atomic number (Z_{eff}) and the electron density (N_{el}),a single number cannot represent the atomic number uniquely across the entire energy range ,as the partial interaction cross –section have different atomic number, Z, dependence[11].

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2.MATHMATICAL BASIS

a) Mass attenuation coefficient:

As a photon makes its path through a matter there is a probability that it makes an interaction with the material such as absorption (photoelectric effect) , scattering (Rayleigh or Compton scattering) or splitting (pair production).Therefore ,part of the incident beam of intensity (I_0) will be partially or completely removed from the beam as a result of interactions within the absorber of thickness x,this reduces the transmitted intensity that reaches the detector to (I) ,where ,introducing the linear attenuation coefficient ,the transmitted intensity is given by ;

$$\mu_L = \ln(I_0 / I)/x \qquad (1)$$

This called the Beer –Lambert law ,where (μ) measured in units of length^{-1} describes the probability of absorption or scattering occurring per unit length within the absorber material [12].The exponential means that equal thickness of the absorber attenuates the photon beam by an equal fraction or percentage [13]. The total mass attenuation coefficient $(\mu/\rho)C$ for any chemical compound or mixture of elements is given by mixture rule [14];

$$(\mu/\rho)_C = \sum_i \omega_i(\mu/\rho)_C \qquad (2)$$

where *wi* and $(\mu/\rho)i$ are the weight fraction and mass attenuation coefficient of the *i*th constituent element, respectively. For a chemical compound the fraction by weight (*wi*) is given by

$$\omega_i = \frac{n_i A_i}{\sum_i n_i A_i} \qquad (3)$$

where *Ai* is the atomic weight of the *i*th element and *ni* is the number of formula units.

b) Cross section :

The cross-section can be defined as the probability of an interaction to occur, it has the dimension of area in units of barn abbreviated *b* = 10-28 m2 = 10-24 cm2 = 100fm2.There are different kinds of cross-sections; atomic, molecular and electronic cross-sections, the atomic cross-section for an element of atomic weight A is given by:

$$\sigma_a = \frac{\mu}{\rho}\frac{A}{N_{av}} \qquad (4)$$

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N_{av} represents the Avogadro's number. For a compound the molecules of which have *ni* atoms for the *i*-th element, the atomic or molecular cross-sections are given by:

$$\sigma_a = \frac{\mu}{\rho}\sum_i \frac{n_i A_i}{\sum n_i}\frac{1}{N_{av}} \qquad (5)$$

The electronic cross-section for an element is given by:

$$\sigma_e = \frac{\sigma_a}{Z} \qquad (6)$$

Hence, for the compound, the electronic cross-section is

$$\sigma_e = \frac{1}{N_{av}}\sum_i \left(\frac{f_i A_i}{Z_i}\right)\left(\frac{\mu}{\rho}\right) \qquad (7)$$

where f_i (= $n_i/\Sigma n_j$) is the fractional abundance of element i, with respect to the total number of atoms. *Zi*: is the atomic number of the element. The effective atomic number (Z_{eff}) is a property for a compound, it describes the properties of the composite materials in terms of equivalent elements, it represents the weighted average atomic number of the compound composed of different materials, the average is weighted according to the relative number of each type of atom, Z_{eff} value of a material varies within a range with lowest and highest atomic numbers of its constituent elements [15].

The effective atomic number is equal to:

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \qquad (8)$$

The electron density can be defined as the number of electrons per unit mass, and it can be mathematically written as:

$$N_{el} = \frac{\left(\frac{\mu}{\rho}\right)_e}{\sigma_e} \qquad (9)$$

where N_{el} represents the electron density in unit of electron/gram, $(\mu/\rho)_c$ is the compound mass attenuation coefficient and σ_e is the electronic cross-section.

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3.SIMULATION

a) MCNP code:

Monte Carlo simulation is found an effective tool to calculate radiation interaction parameters in different types of compounds and mixtures for shielding and energy deposition in human organs and tissues. MCNP is a general purpose Monte Carlo code for transport of neutrons, photons and electrons. The user can apply up to second order surfaces (boxes, ellipsoids, cones, etc.) and fourth order torii to build a 3D geometry which can be filled with materials of arbitrary composition and density. Point, surface or volume sources of radiation can be defined, from which the mentioned particles are emitted with user specified probability distributions for energy and direction.The code then simulates the particle tracks and interactions with the materials, according to probability density distributions [16].

b) XCOM software:

The μ/ρ values of biological samples were calculated by mixture rule $(\mu/\rho)_C = \sum_i \omega_i (\mu/\rho)_i$ where *wi* is the proportion by weight and $(\mu/\rho)_i$is mass attenuation coefficient of the i^{th} element by using XCOM [17]. The uncertainties in μ/ρ values is about 1% for low-Z (1<Z<8) in Compton region (30 keV to 100 MeV). 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. Below 30 keV energy, the uncertainties are as much as 5-10% because of correction to experiments for high-Z impurities and departure of Compton cross section from Klein-Nishina theory. Also above 100 MeV photon energy, uncertainties in μ/ρ values may be 5-10%.Uncertainties in photon energy absorption coefficient may be slightly greater values [18]. The gamma sources of photon energies above 5keV are being used in medical, biological, industrial, radioactive source transportation and other shielding applications. Hence uncertainty in the result may not have any impact for practical applications.

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4.RESULTS AND DISCUSSION

A) Calculation Linear attenuation coefficients in ionic crystals:

Figures (1-4) Illustrate linear the relationship between the the logarithm values linear gamma rays of different energies and with thickness proposed model .Calculate the amount of the linear attenuation coefficient for each of the ionic crystals by drawing the relationship between the ratio of the $\ln(I_0 / I)$ with thickness materials, was get a straight line slope is equal to the value of the linear attenuation. From Table (1) and Figure (5) shows There exponential relationship between the linear attenuation coefficient and photon energy.In any case to see mass attenuation depend in atomic number and energy gamma. It is clear that there is satisfactory agreement between Monte Carlo and XCOM program ,although the Monte Carlo values tend to be larger than the the XCOM values .

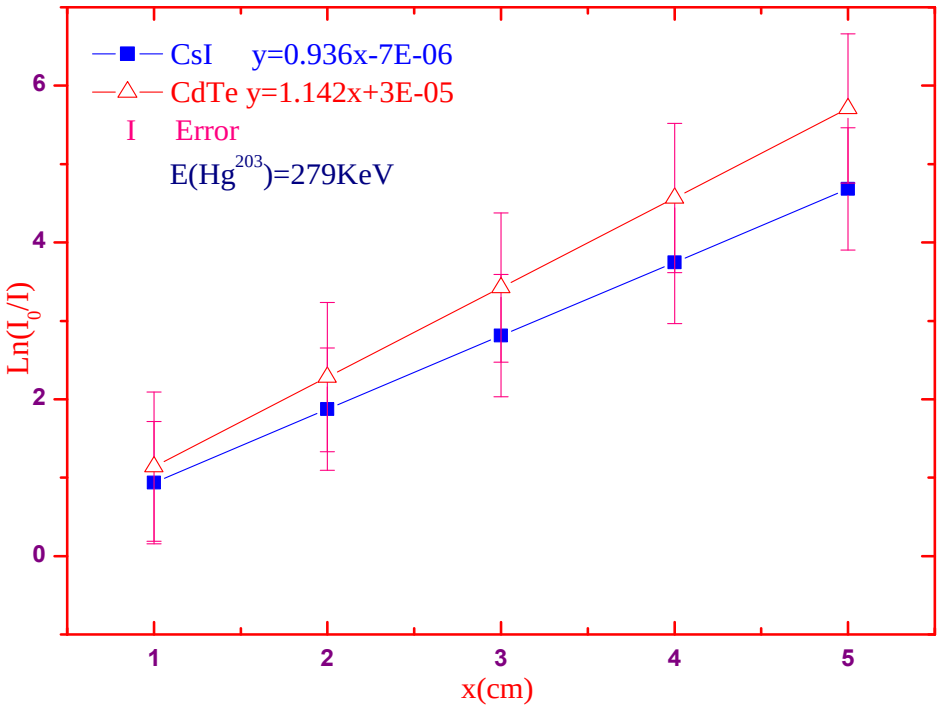

Figure (1): shows the relationship between the logarithm of the absorbance of gamma ray energy (279 KeV) and thickness for ionic cryatals.

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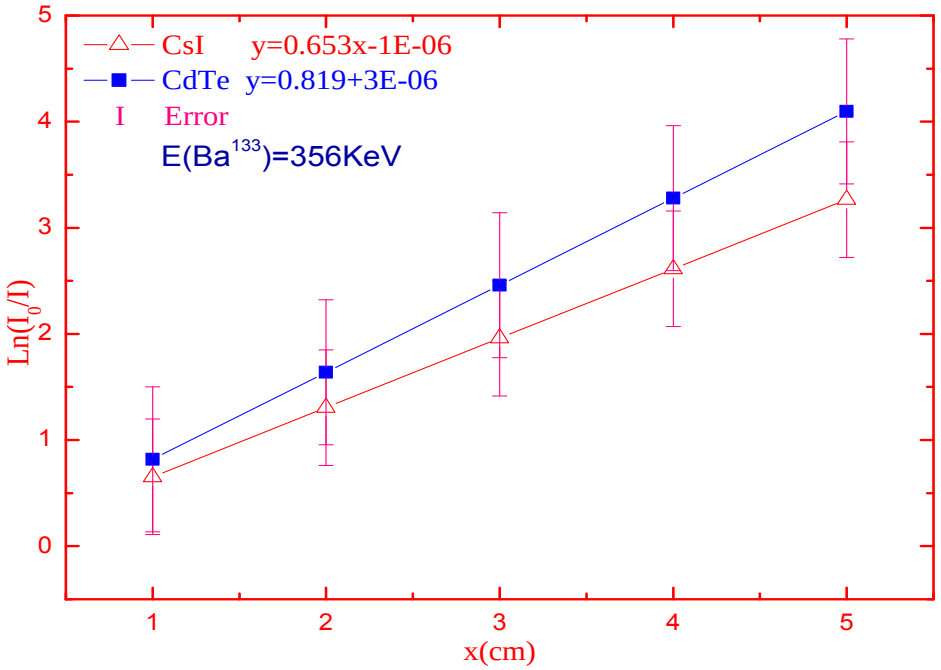

Figure (2): shows the relationship between the logarithm of the absorbance of gamma ray energy (356 KeV) and thickness for ionic crystals'.

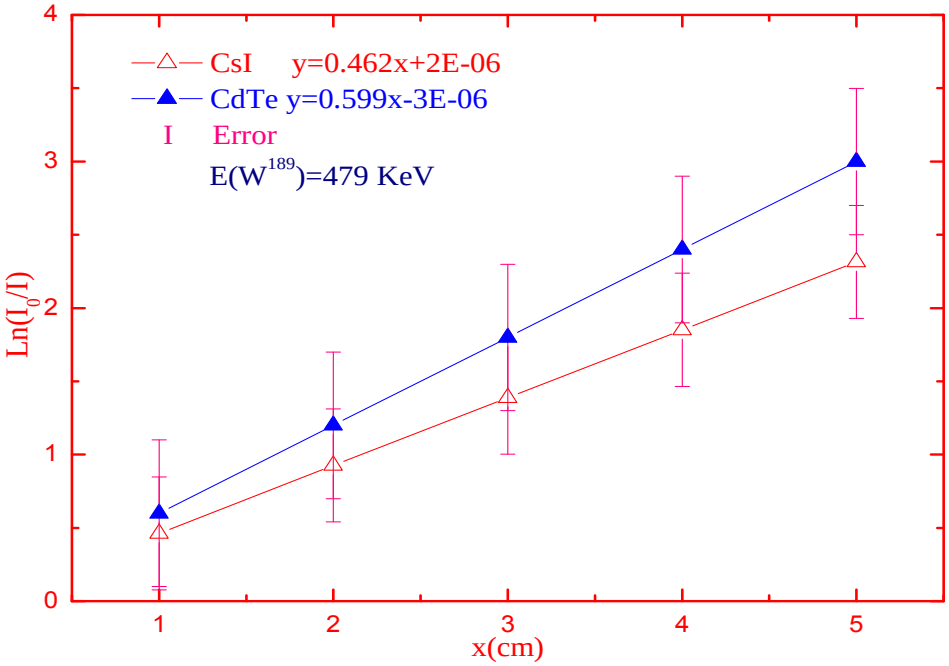

Figure (3): shows the relationship between the logarithm of the absorbance of gamma ray energy (479 KeV) and thickness for ionic crystals'.

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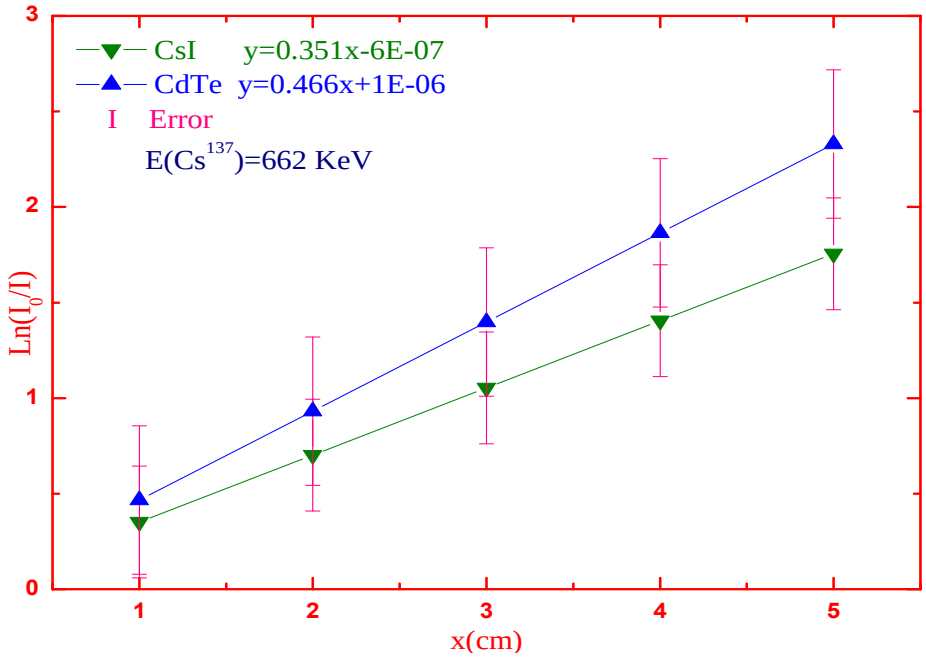

Figure (4): shows the relationship between the logarithm of the absorbance of gamma ray energy (662 KeV) and thickness for ionic crystals'.

Table (1): Shows a comparison between the calculated values (μ_L) of the Monte Carlo program with the calculated values of the program (XCOM) within the range of energies.

E(KeV)	CsI		CdTe	
	μ_L(cm^{-1}) present work	μ_L(cm^{-1}) *Xcom*	μ_L(cm^{-1}) present work	μ_L(cm^{-1}) *Xcom*
279	0.936	0.9254	1.142	1.1253
356	0.653	0.643	0.819	0.812
479	0.462	0.460	0.599	0.597
662	0.351	0.348	0.466	0.462

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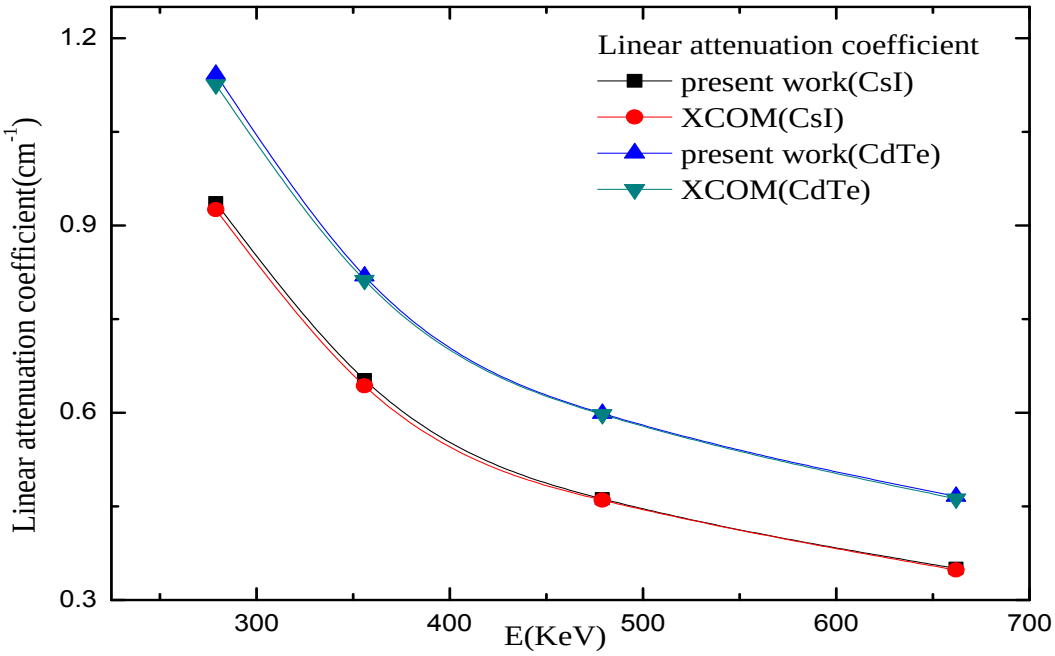

Figure (5): Illustrates the exponential relationship between the linear attenuation coefficient and the photon energy of ionic crystals calculated by the Monte Carlo program and XCOM package.

B) Calculation Mass attenuation coefficients in ionic crystals:

Mass attenuation coefficients for (CsI and CdTe) studied in the present work have been obtained using Monte Carlo simulation for different photon energies. The values obtained theoretically are compared with the values results from XCOM package, Observe there was good agreement between the results as seen in the table (2).The mass attenuation coefficient values decrease with increase in photon energy as seen from figure (6) .The calculated values for almost the ionic crystals studied in the present work are higher than their XCOM results.

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Table (2): Shows a comparison between the calculated values (μ_m) of the Monte Carlo program with the calculated values of the program (XCOM) within the range of energies.

E(KeV)	CsI		CdTe	
	μ_m(cm^2/gm) present work	μ_m(cm^2/gm) *XCOM*	μ_m(cm^2/gm) present work	μ_m(cm2gm) *XCOM*
279	0.2077	0.2052	0.1842	0.1815
356	0.1449	0.1427	0.1322	0.1308
479	0.1026	0.1021	0.0968	0.09633
662	0.0779	0.07722	0.0752	0.07459

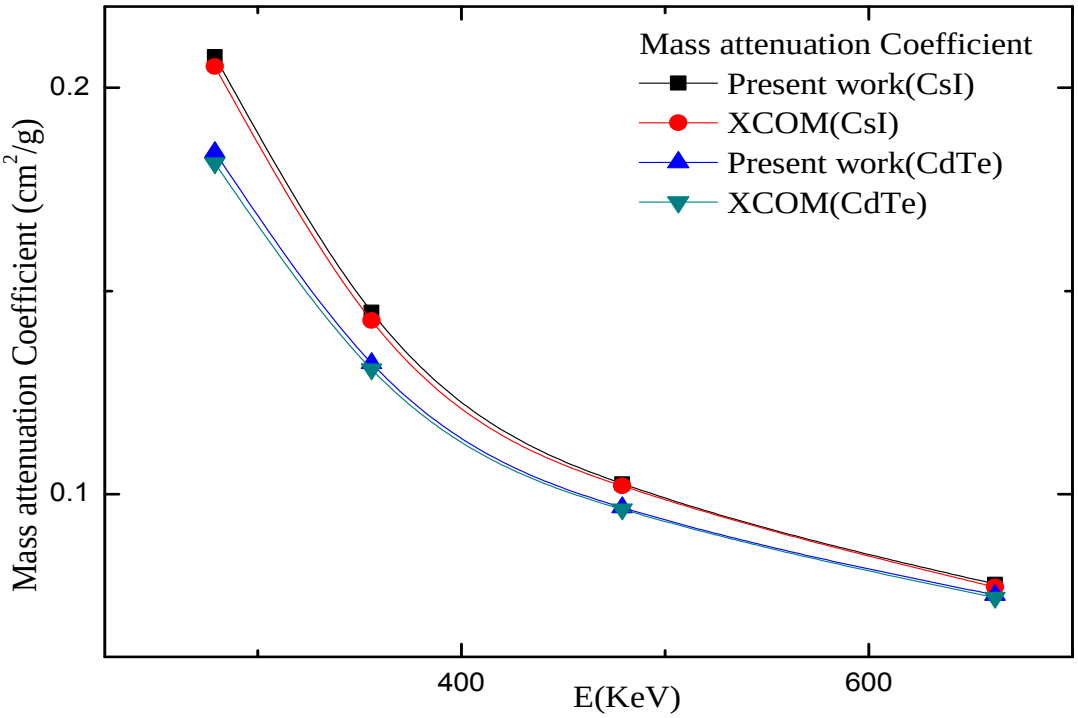

Figure (5): Illustrates the exponential relationship between the linear attenuation coefficient and the photon energy of ionic crystals calculated by the Monte Carlo program and XCOM package.

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C) Calculation total atomic cross section and electron density:

Measured total atomic and electronic cross section for ionic crystals were presented in Table (3&4).The variation of σ_t and σ_e to observe almost similar behavior to linear attenuation and mass attenuation .Atomic and electronic cross section values decrease because probability of absorption reduce with increasing incident photon energies. From Table (5&6) the electron density and effective atomic number remains constant and are found to be independent of photon energy for two samples. It was observed that the simulation processes using MCNP were in good agreement with the results values from XCOM.Z_{eff} value for composite material is very useful parameter for some applications such as physical ,technological and engineering .Z_{eff} represented with a number provides many characteristics of a material .For example ,Z_{eff} value can provide estimation of the chemical composition of the material and it can be also utilized in the computation of absorbed dose in radiation therapy etc. In this study ,Z_{eff} values were determined from Eqs(5-8) by using the (μ_m) values , and given in Table (6).

Table (3): The atomic cross section for CsI and CdTe calculation by Monte Carlo program and with XCOM program.

E (KeV)	CsI		CdTe	
	(σ_a) $cm^2/atom$		(σ_a) $cm^2/atom$	
	present work	$XCOM$	present work	$XCOM$
279	4.48028E-23	4.42635E-23	3.67071E-23	3.6169E-23
356	3.12562E-23	3.07817E-23	2.63446E-23	2.60656E-23
479	2.21318E-23	2.20239E-23	1.92902E-23	1.91965E-23
662	1.68037E-23	1.66571E-23	1.49857E-23	1.48642E-23

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Table (4): The electronic cross section for CsI and CdTe calculation by Monte Carlo program and with XCOM program.

E (KeV)	CsI (σ_e) $cm^2/atom$		CdTe (σ_e) $cm^2/atom$	
	present work	*XCOM*	present work	*XCOM*
279	8.29067E-25	8.19088E-25	7.31508E-25	7.20786E-25
356	5.78391E-25	5.69609E-25	5.25002E-25	5.19443E-25
479	4.09544E-25	4.07548E-25	3.84419E-25	3.82553E-25
662	3.1095E-25	3.08236E-25	2.9864E-25	2.96217E-25

Table (5): The electronic density for CsI and CdTe calculation by Monte Carlo program and with XCOM program.

E (KeV)	CsI (N_{el})electron/gram		CdTe (N_{el})electron/gram	
	present work	*XCOM*	present work	*XCOM*
279	2.50523E+23	2.50523E+23	2.51808E+23	2.52E+23
356	2.50523E+23	2.50523E+23	2.51808E+23	2.52E+23
479	2.50523E+23	2.50523E+23	2.51808E+23	2.52E+23
662	2.50523E+23	2.50523E+23	2.51808E+23	2.52E+23

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Table (6): Show effective atomic number for CsI and CdTe calculation by Monte Carlo program and with XCOM program.

E (KeV)	CsI		CdTe	
	Z_{eff}		Z_{eff}	
	present work	*XCOM*	present work	*XCOM*
279	54.04	54.04	50.18	50.18
356	54.04	54.04	50.18	50.18
479	54.04	54.04	50.18	50.18
662	54.04	54.04	50.18	50.18

5.CONCLUSION

In this study, the Monte Carlo code was used for calculation of (μ_L, μ_m) , total atomic cross section ,electronic cross section ,electron density and effective atomic number for (CsI, CdTe) in the photon energy (279, 356, 479, 662)KeV.In this paper understand that the μ_m is useful and sensitive physicsl quantity to determine the $\sigma_t, \sigma_e, Z_{eff} and\ N_{el}$ for ionic crystals. From the data , CdTe appears as agood attenuater ,and the inverse relation between energy and gamma attenuation clearly appears. Also observe attenuation coefficient for CdTe higher than from CsI .

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