Effective atomic number and electron densities of some alkali halides for wide energy region by using mass attenuation coefficients

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Abstract

Effective atomic numbers (Z_{eff}) and electron densities (N_{el}) of some alkali halides CuCl, RbI and CsBr have been calculated for the total and partial photon interactions. The mass attenuation coefficients for the wide energy range 1 keV-100 GeV has been obtained from WinXCom. Variation of mass attenuation coefficients as a function of energy are shown graphically. The maximum values of Zeff and Nel are found in the low-energy range, where photoelectric absorption is the main interaction process. Compton scattering is the main interaction process in intermediate energy region. At high energies, pair production is the main dominating interaction process. The average values of Zeff and Nel have been also calculated for photoelectric absorption, coherent, incoherent, pair production in the field of electric and nuclear. It has been observed that Zeff and Nel values vary as energy varies, they are not true constants of the material.

• Introduction

The mass attenuation coefficient or mass extinction coefficient of the volume of a material characterizes how easily it can be penetrated by a beam of light, particles or other energy or matter. In addition to visible light, mass attenuation coefficient can be defined for other electromagnetic radiation (such as X-rays) or any other beam that attenuates [1]. The SI unit of mass attenuation coefficient is the square meter per kilogram [2, 3]. The mass attenuation coefficient can be thought of as a variant of absorption cross section where the effective area is defined per unit mass instead of per particle. The attenuation coefficient is defined as the probability of a radiation interacting with a material per unit path length [4]. Linear attenuation coefficient for a material depends on the incident photon energy, the atomic number and the density of material [5].

Effective atomic number (Z_{eff}) has two different meanings: one that is the effective nuclear charge of an atom and one that calculates the average atomic number for a compound or mixture of materials both are abbreviated Z_{eff}. As stated by Hine [6], for gamma photon interactions a single number cannot represent the “effective” atomic number of a multi element material, composed of several elements, uniquely across the entire energy region. Instead, one defines the

so-called effective atomic number, Z_{eff}. for each of the different processes, by which X-rays or gamma rays [7] can interact with matter, the various atomic numbers in the material have to be weighted differently. In general, the effective atomic number is large for inorganic compounds and metals while it is small for indicator of organic substances. Among the parameters representing radiation interaction with materials, it should be noted that Z_{eff} is one of the most convenient parameter [8]. The other important quantity is the effective electron number or electron density and it is defined as the electrons per unit mass of the absorber [9].

The Berger and Hubbel [10] developed a computer program XCom, for calculating mass attenuation coefficients and cross-section. For any element, compound and mixture at the energies 1 keV to 100 GeV. This is well-known and widely used program was enhanced and transformed to the windows platform by Gerward et al [11] and it is known as WinXCom. The effective atomic number of organic molecules like radioactive isotopes and organic liquid scintillators play an important role in the biological and pharmaceutical field [12, 13]. The mass attenuation coefficients, effective atomic cross sections [14, 15], effective atomic numbers and electron densities of some halides were determined by Shivalinge Gowda [16]. The total mass attenuation coefficients μ/ρ, of some alkali halides were determined for selected photon energies in a well-collimated narrow beam good geometry set-up using a high resolution, hyper pure germanium detector. This prompted us to study the mass attenuation coefficients, effective atomic numbers and electron densities of selected halides such as CuCl, RbI and CsBr. I have used direct method to calculate Z_{eff} among different methods such as Interpolation method, Auto Z_{eff} method [17] and Single value XMuDat computer program [18, 19].

In the present work, mass attenuation coefficients and interaction cross-sections of the elements and materials were generated using the computer program WinXCom. The effective atomic number and electron densities have been calculated for Alkali halides CuCl, RbI and CsBr for all photon interactions [coherent, incoherent, photoelectric, pair production, total photon interaction (with coherent and incoherent)] in the energy range 1 keV-100 GeV using WinXCom Program. The variations of effective atomic number and electron density with energy are shown graphically for all total photon interaction.

2. Theoretical basis

The calculation methods for the effective atomic numbers electron density and Kerma of alkali halides are described in the following subsections.

2.1 Mass attenuation coefficients

The total photon mass attenuation coefficient for a chemical compound or mixture was calculated using the WinXCom and the following ‘mixing rule’ [20] .

$$\left(\frac{\mu}{\rho}\right)_{comp} = \sum_i \omega_i \left(\frac{\mu}{\rho}\right)_i \quad (1)$$

where and are the photon mass attenuation coefficient and the weight fraction of the i^{th} constituent element in the compound, respectively.

$$\omega_i = \frac{n_i A_i}{\sum_i n_i A_i} \quad (2)$$

where is the ith element's atomic weight and is the number of formula units in i^{th} element [21].

2.2 Effective atomic numbers

Calculation of the effective atomic numbers Z_{eff}, PI of the low-Z materials for total photon interaction was carried out by using practical formula. The formula is given below [22]:

$$Z_{eff,pl} = \frac{\sum_i f_i A_i (\mu/\rho)_i}{\sum_j (f_j A_j / Z_j)(\mu/\rho)_j} \quad (3)$$

where is molar fraction in the mixture/compound, is linear attenuation coefficient, is density, is mass attenuation coefficient, is atomic weight, is atomic number and the ratio, between the atomic mass and the atomic number is approximately constant.

2.3 Electron density

The effective electron density N_{el} (number of electrons per unit mass) is derived as:

$$N_{el} = \frac{N_A}{\sum_i A_i n_i} Z_{eff} = \frac{N_A}{\langle A \rangle} Z_{eff} \quad (4)$$

where <A> average atomic mass of the compound.

Theoretical values for the mass attenuation coefficient can be found in the tabulation by Hubbell and Seltzer [23]. Instead of interpolating tabulated values and using the mixture rule, some computer programs such as WinXCom can save a lot of manualworkando

3. Results and discussions

3.1 Mass attenuation coefficients

Mass attenuation coefficient and attenuation cross-section data are available in photon energy range of 1 keV to 100 GeV in the XCOM program which has been transformed to windows operating system software WinXCom [26] . Effective atomic numbers are derived by calculation of the mass attenuation coefficients [18] and atomic cross-sections of the elements of compound/mixture. The elemental compositions of the high-Z materials [27] used in this study are given in Table 1. For total photon interaction process (with coherent), the variation of mass attenuation coefficient against optical energy of the compounds obtained by WinXCom is shown in Fig. 1. The variation of mass attenuation coefficient is different for the alkali halides at various energies. Photoelectric absorption, Compton scattering and pair production are the three dominant attenuation mechanisms, as shown in the graph. Photoelectric effect is the main

interaction process from 1 keV upto 5 keV, 50 keV and 200 keV for CuCl, RbI and CsBr respectively. At intermediate energies Compton scattering is interaction dominant process. At high energies above 100 MeV pair production will become the dominating interaction process [28].

Table 1 The molecular formula for Alkali halides.

S.NO.	Name of Compound	Molecular Formula
1.	Calcium Chloride	CuCl
2.	Rubidium iodide	RbI
3.	cesium Bromide	CsBr

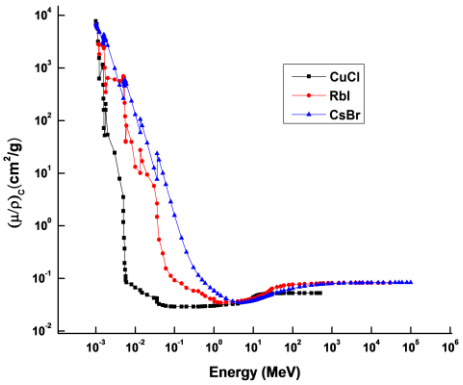


FIG. 1 Variation of photon mass attenuation coefficient (μ/ρ) of alkali halides with photon energy for total photon interaction (with coherent).

3.2 Effective atomic number and electron density

a) Total photon interaction (with coherent and incoherent)

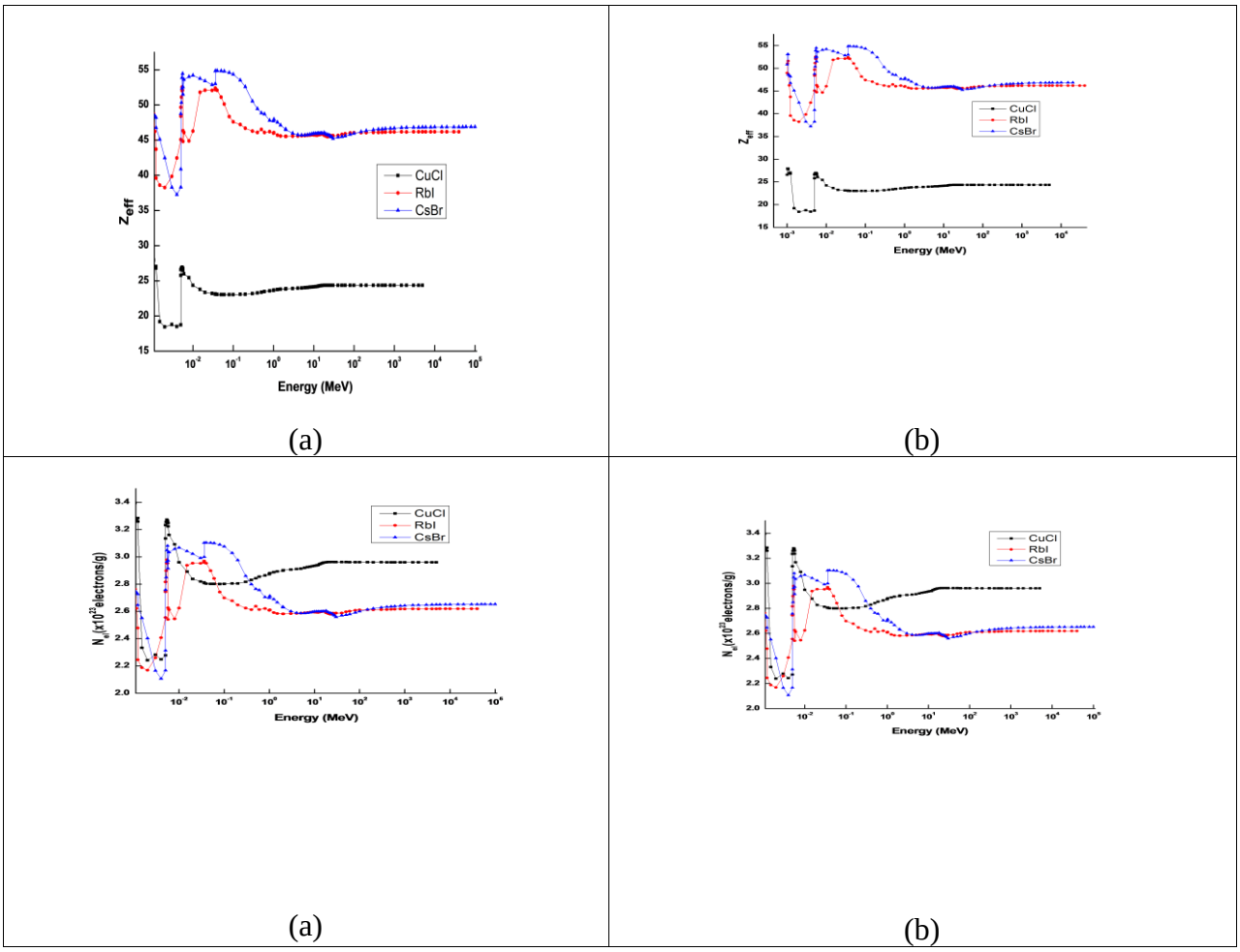


FIG. 2 Energy dependence of Z_{eff} and N_{el}, of alkali halides for total photon interaction (a) with coherent and (b) with incoherent.

The Z_{eff} and N_{el} of alkali halides were calculated using mass attenuation coefficients of chemical composition of the given molecule or compound. From Fig. 2 (a & b) it can be seen that the Z_{eff} and N_{el} are mainly dominated by different partial photon interaction processes [29]. The value of average effective atomic number $<Z_{eff}>$ and electron density $<N_{el}>$, have been shown in the Table 2, 3 and 4. The Z dependency of total atomic cross–sections explains all changes, leading to effective atomic numbers such as Z^{4-5} for photoelectric absorption, Z for Compton scattering and Z^2 for pair production [30]. The Z_{eff} varies from a higher value at lower energies to a lower value at higher energies, with a peak due to photoelectric effect near the K-edge of the high Z element present in alkali halides. The Maximum values of Z_{eff} were found for RbI and

Table 2 Average of effective atomic numbers and electron densities (10^{23}electrons/gram) of Alkali halide material (CuCl).

Name of the process	$\langle Z_{eff} \rangle$	$\langle N_{el} \rangle$
Total non-coherent	24.19	2.94
Total coherent	24.19	2.94
Pair electron	23.68	2.88
Pair nuclear	24.98	3.037
Photo electric	27.87	3.39
Incoherent	24.91	3.03
Coherent	27.62	3.36

Table 3 Average of effective atomic numbers and electron densities (10^{23} electrons/gram) of Alkali halide material (CsBr).

Name of the process	$\langle Z_{eff} \rangle$	$\langle N_{el} \rangle$
Total non-coherent	48.01	2.73
Total coherent	47.96	2.71
Pair electron	44.41	2.51
Pair nuclear	46.31	2.62
Photo electric	53.27	3.01
Incoherent	49.47	2.80
Coherent	53.34	3.02

Table 4 Average of effective atomic numbers and electron densities (10^{23} electrons/gram) of Alkali halide material (RbI).

Name of the process	$\langle Z_{eff} \rangle$	$\langle N_{el} \rangle$
Total non-coherent	46.61	2.64
Total coherent	46.62	2.64
Pair electron	45.01	2.55
Pair nuclear	46.29	2.62
Photo electric	50.62	2.87

Incoherent	47.51	2.69
Coherent	50.64	2.87

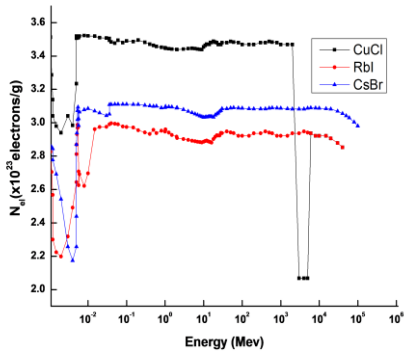
CsBr than CuCl due to the presence of high Z elements. Energies below 5 keV, 30 keV and 60 keV for the three alkali halides photoelectric absorption is dominant. After those energies Compton scattering will become the dominant interaction process, between energies 15 keV-300 keV, 400 keV-100 MeV. Z_{eff} and N_{el} becoming constant with a minimum value at intermediate energies; further, there is an increasing trend in Z_{eff} values due to the relative dominance of photon interaction processes in various energy regions. From 100-200 MeV pair production starts becoming dominating process. After 200 MeV Z_{eff} will become energy independent [31, 35].

b) Photoelectric absorption

A plot of Z_{eff} vs photon energy, especially for medium and high-Z materials, shows the distinctive K absorption edges [36]. This is because; photoelectric process is predominant at low energies (1 MeV) and for materials of higher atomic numbers. Fig 3 (a and b) demonstrate the fluctuation of Z_{eff} and N_{el} with photon energy for photoelectric absorption. After 5 keV, Z_{eff} and Nel become almost constant [37, 38].

c) Coherent & incoherent scattering

The Fig. 3 (a and b) shows the variation of Z_{eff} and N_{el} with photon energy for coherent scattering. It is observed from the figures that Z_{eff} is independent of energy. Similarly, the variation of Z_{eff} with photon energy for incoherent scattering is shown in Fig. 4 (a and b) which indicates that Z_{eff} is constant in the energy region 1 keV–100 GeV [39].



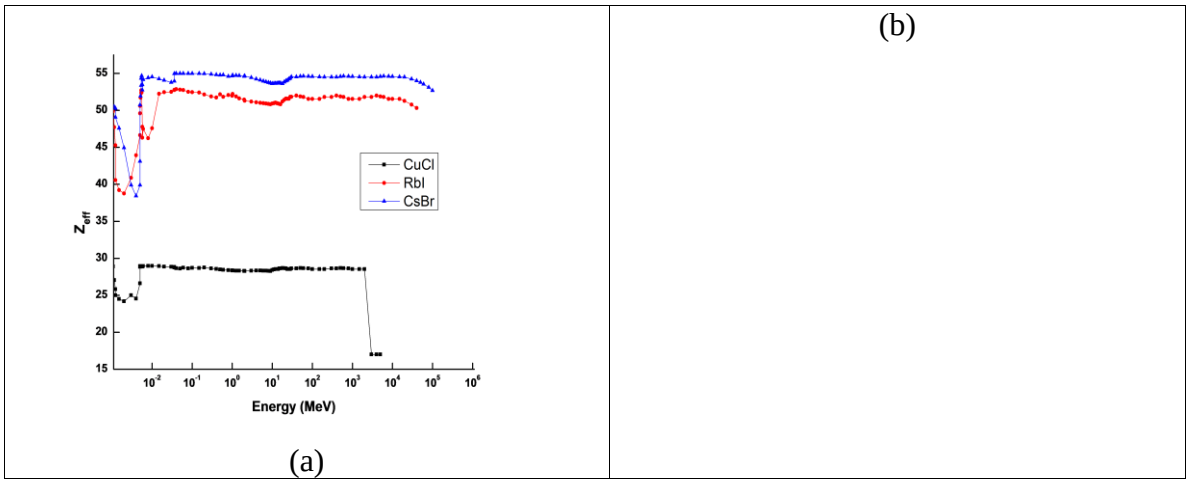


FIG. 3 Energy dependence of Z_{eff} and N_{el}, of alkali halides for photoelectric absorption.

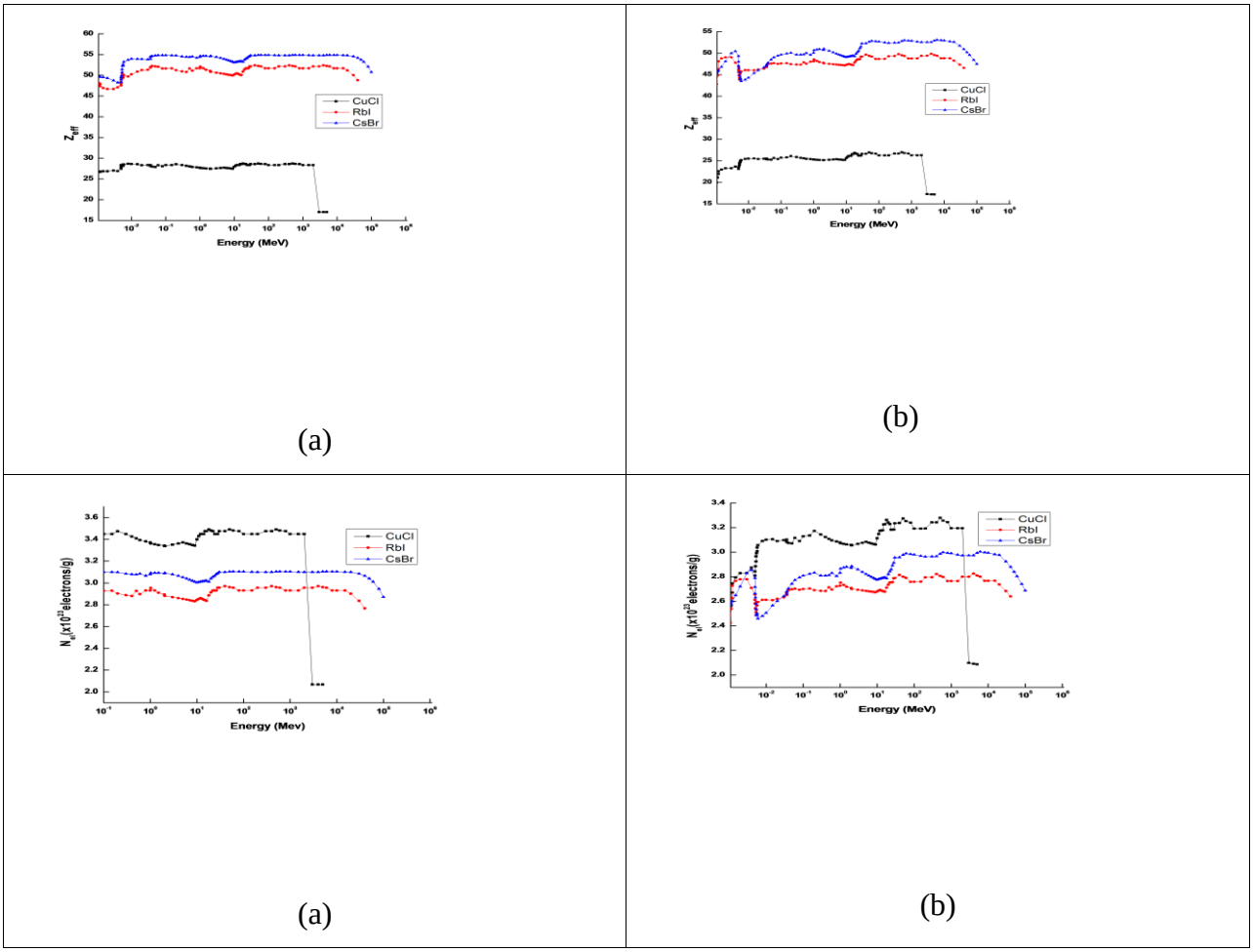


FIG. 4 Energy dependence of Z_{eff} and N_{el}, of alkali halides for (a) coherent and (b) incoherent

d) Pair production in nuclear field and electric field

The variation of Z_{eff} with photon energy for electric field is shown in Fig. 5 (a and b), which demonstrates that Z_{eff} increases significantly with increasing photon energy from 100 keV-1 MeV
for CuCl and from 1 MeV-30 MeV for RbI and CsBr before becoming energy independent. It could be because pair production in the nuclear field is Z^2 dependent. The variation of Z_{eff} and N_{el} with photon energy for Pair production in the nuclear field is shown in Fig. 4 (a and b). The variation is nearly same for as that of electric field [40, 41], .

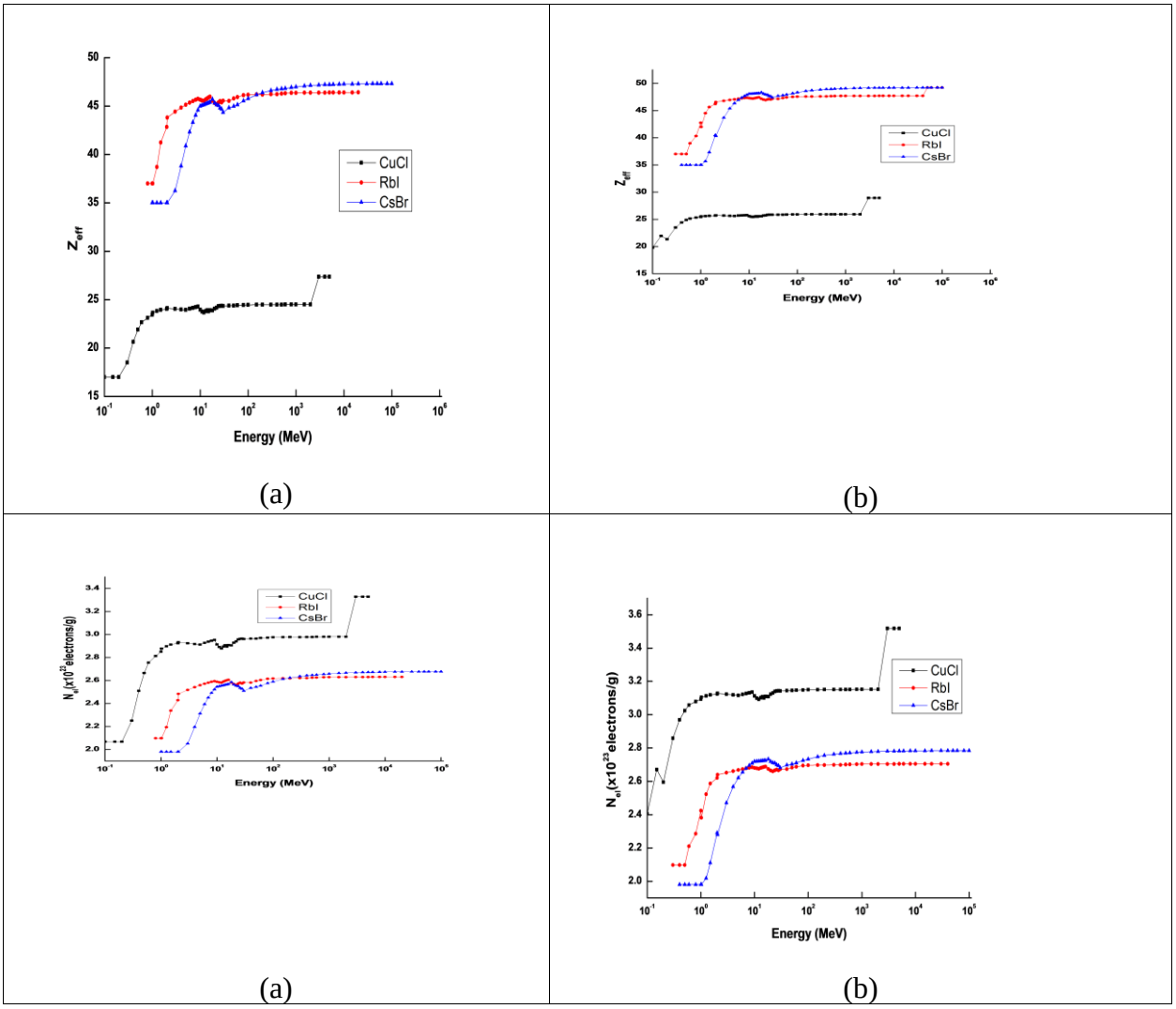


FIG. 5 Energy dependence of Z_{eff} and N_{el}, of alkali halides for pair electric and (b) pair nuclear field.

Conclusions

The effective atomic number Z_{eff} and electron density N_{el} of alkali halide CuCl, RbI and CsBr has been calculated in the extended energy region from 1 keV-100 GeV using WinXCom program. In total photon interaction with coherent and incoherent one can distinguish three energy regions. The main photon interaction processes in these regions are photoelectric absorption, incoherent (Compton) scattering and pair production. Z_{eff} and N_{el} values have also been calculated for different processes such as pair production in nuclear and electric field, photoelectric absorption, coherent and incoherent scattering. The maximum values of Z_{eff} and N_{el} are found in the low energy range, where photoelectric absorption is the main interaction process. The minimum values of Z_{eff} and N_{el} are found at intermediate energies, where Compton scattering is dominant. At high energies Z_{eff} and N_{el} are independent of the energy. This may be due to the dominance of pair production in the high energy region.

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