# Effective atomic number and electron density of some organic molecules containing C, H, N and O atoms

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## Abstract

The effective atomic number ($Z_{eff}$) and electron density ($N_{el}$) of organic molecules viz., benzofuran and coumarin derivatives have been calculated in the extended energy range 1 keV-100 GeV using photon interaction cross section data base and WinXCom program. The variation of $Z_{eff}$ and $N_{el}$ values with energies are represented graphically and the variation of both parameters, $Z_{eff}$ and $N_{el}$ with energies is same.The considerable variation in $Z_{eff}$ and $N_{el}$ is due to the dominance of different interaction mechanisms in that energy region, such as photoelectric absorption, Compton scattering and pair creation.

**Key words:** Effective atomic number, electron density, organic molecules, XCom
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## Introduction

The photon mass attenuation coefficient, effective atomic number and electron density are the basic quantities required in determining the penetration of X-rays and gamma photons in matter. The mass attenuation coefficient (μ/ρ) is a measure of probability of interaction that occurs between incident photons and matter per unit areaG. J. Hine has pointed out that in composite materials, for photon interactions, a single number cannot represent the atomic number uniquely across the entire energy region, as in the case of pure elements [1]. This number for composite materials is known as “effective atomic number ($Z_{eff}$) and it varies with energy. The energy absorption in a given medium can be calculated if certain constants are known. These necessary constants are $Z_{eff}$and electron density $N_{el}$ of the medium.

As effective atomic numbers and electron densities are useful in many technological applications, several investigators have made extensive studies of effective atomic numbers in variety of composite materials like alloys, polymers compounds, and mixtures, thermo luminescent dosimetriccompounds, semiconductors and superconductors. The effective atomic number $Z_{eff}$ has an interesting application which can be used in security screening of air passenger luggage for organic molecules, in particular for substance of low crystalline.

There are almost noreports on the effective atomic number and electron density studies of organic molecules which we have selected in this present work. This prompted us to study the mass attenuation coefficient (μ/ρ) and hence effective atomic number $Z_{eff}$ and electron density $N_{el}$.

In the present work, the effective atomic number and electron densities have been calculated for for all photon interactions (with coherent) of the organic molecules in the energy range 1Kev-100GeV using WinXCom program [2, 3]. The variations of effective atomic number and electron density with energy are shown graphically for the all photon interactions.

## Computational methods

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

$$Z_{eff,pl} = \frac{\sum_i f_i A_i (\mu/\rho)_i}{\sum_j (f_j A_j / Z_j)(\mu/\rho)_j} \tag{1}$$

Where fi is molar fraction in the mixture/compound, μ is linear attenuation coefficient, ρ is density, μ/ρ is mass attenuation coefficient, A is atomic weight, Z is atomic number, and the ratio, A/Z, between the atomic mass and the atomic number is approximately constant.

## Electron density

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

$$N_{el} = \frac{(\mu/\rho)_c}{a_c} = \frac{N_A}{M} Z_{eff} \sum_i n_i \tag{2}$$

Theoretical values for the mass attenuation coefficient can be found in the tabulation by Hubbell and Seltzer .Instead of interpolating tabulated values and using the mixture rule, some computer programs such as WinXCom or its predecessor XCOM can save a lot of manual work and of course time [4].

## Results and discussions

In the present work, the variations of $Z_{eff}$and $N_{el}$ with photon energy for organic molecules composed of different elements in different proportions (Table 1) were studied. The results are shown graphically for partial and total photon interaction processes. The $Z_{eff}$and $N_{el}$values of organic drug (morphine and Methadone) are given in (Table 1)only for total photon interaction. The present results clearly confirm the comment made by Hine mentioned earlier that the effective atomic number varies with energy. In the following paragraphs energy dependence of $Z_{eff}$ and $N_{el}$ for total and individual photon interactions are involved.



**Table 1:** The molecular formula for organic molecules.

| Name of Compound | Molecular Formula | $\langle Z_{eff} \rangle$ | $\langle N_{el} \rangle$ |
|---|---|---|---|
| Morphine | $C_{17}H_{19}NO_3$ | 6.36 | 6.42 |
| Methadone | $C_{21}H_{27}NO$ | 5.86 | 6.33 |

## Total photon interaction (with coherent)

From the figure it can be easily seen there are three energy ranges where photoelectric absorption, Compton scattering and pair production, respectively, visual photon interactions are discussed. These variations are interpreted as being due to photoelectric effect which varies as $Z^{4-5}$ and less but significantly due to coherent scattering which varies as $Z^{2-3}$. This fact has been verified experimentally by singh by measuring total mass attenuation coefficient of some soils. The present theoretical results are similar to the observations of Zavelski who proposed a direct relation of (μ/ρ) with heavy metals in the rock salt at low energy. In the intermediate energy region, where incoherent scattering is the most dominant process.

Mass attenuation coefficient is found to be constant and is due to the linear Z-dependence of incoherent scattering and insignificant role played by pair production. In the high energy region, the variation in mass attenuation coefficient is due to the $Z^2$-dependence of pair production. The variation of$Z_{eff}$ with photon energy for total photon interaction the dominance of different interaction process in different energy regions. In low energy region photoelectric interaction is dominant; $Z_{eff}$ varies as in case of photo interaction process 8keV on wards there is a sharp decrease in $Z_{eff}$ with energy up to 150keV, showing that contribution of scattering processes increases which decreases $Z_{eff}$. This is also confirmed by confirmed that $Z_{eff}$ of composite material for photoelectric interaction is great [5].

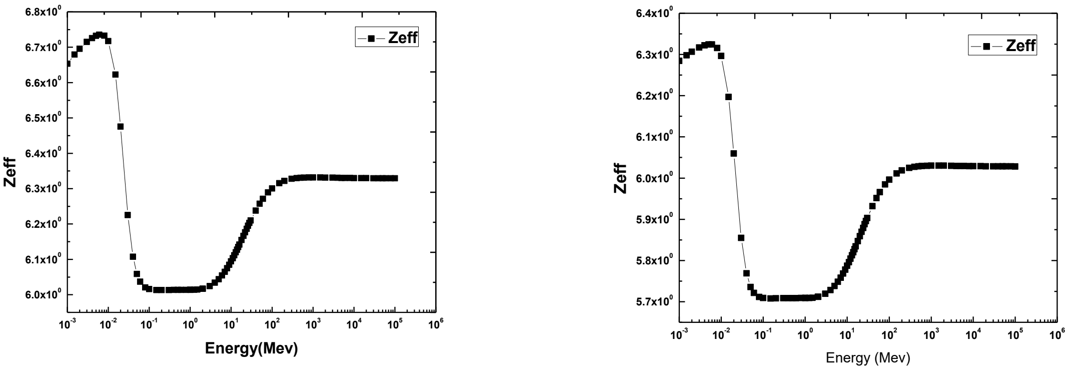


**Fig 1:** Variation of effective atomic number $Z_{eff}$ of Morphine and Methadone with photon energy for total incoherent $Z_{eff}$

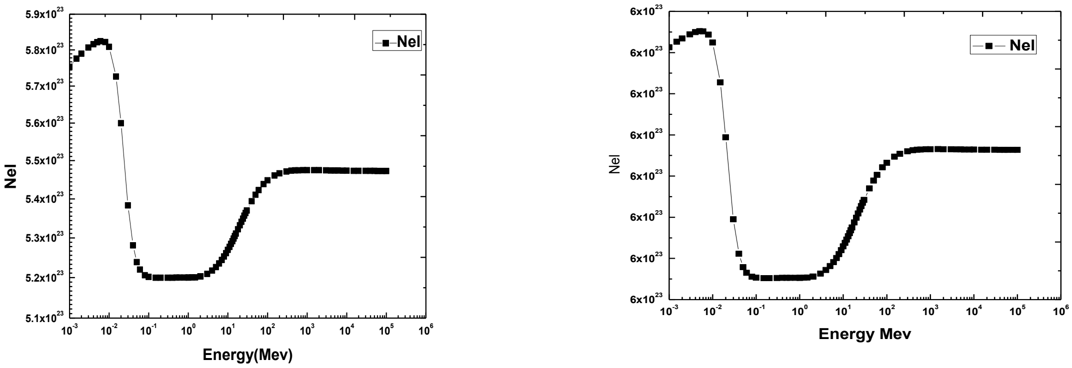


**Fig 2:** Variation of effective atomic number $N_{el}$ ofMorphine and Methadone with photon energy for total coherent

The variation of $Z_{eff}$ and $N_{el}$ values with energies are represented graphically and the variation of both parameters, $Z_{eff}$ and $N_{el}$ with energies is same.The variation in $Z_{eff}$ and $N_{el}$ is due to the dominance of different interaction processes in that energy region1 keV-100 GeV,such as photoelectric absorption, Compton scattering, and pair creation [6].

**Conclusions**

The Effective atomic number and electron density of few organic molecules such as, Methadone ($C_{21}H_{27}NO_3$),Morphine($C_{17}H_{19}NO_3$) have been calculated for total and partial photon interactions by the direct method in the wide energy range of 1keV -100GeV using WinXCom. These are especially used in medicine, agriculture, industry, security screening etc.

**References**

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