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Calculation of Absorption Parameters for Selected Narcotic Drugs in the Energy Range from 1 keV to 100 GeV

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Abstract. The total mass attenuation coefficients (μ/ρ), total molecular ($\sigma_{t,m}$), atomic ($\sigma_{t,a}$) and electronic ($\sigma_{t,e}$) cross sections, effective atomic numbers (Z_{eff}) and electron density (N_E) were computed in the wide energy region from 1 keV to 100 GeV for the selected narcotic drugs such as morphine, heroin, cocaine, ecstasy and cannabis. The changes of μ/ρ, $\sigma_{t,m}$, $\sigma_{t,a}$, $\sigma_{t,e}$, Z_{eff} and N_E with photon energy for total photon interaction shows the dominance of different interaction process in different energy regions. The variations of μ/ρ, $\sigma_{t,m}$, $\sigma_{t,a}$, $\sigma_{t,e}$, Z_{eff} and N_E depend on the atom number, photon energy and chemical composition of narcotic drugs. Also, these parameters change with number of elements, the range of atomic numbers in narcotic drugs and total molecular weight. These data can be useful in the field of forensic sciences and medical diagnostic.

INTRODUCTION

The term "narcotic" is imprecisely defined and typically has negative association of ideas. Narcotic drugs are completely interdicted and they can be used with special permissions. The term "narcotic" actually intends medically to any psychoactive compound with sleep-inducing properties. In this study, the discussed narcotic drugs are; morphine, heroin, cocaine, ecstasy and cannabis.

The absorption parameters such as total mass attenuation coefficient, effective atomic number and electron density are needed to be determined precisely in atomic physics, medical diagnosis, agriculture, industry, space physics, radiation physics and surface and material sciences. The mass attenuation coefficient is the most fundamental parameter to study the interaction of photon with matter within these absorption parameters. The mass attenuation coefficient that is a measure of probability of interactions of photons with matter. The quantity "effective atomic number" has a physical meanings and allows many characteristics of a matter to be visualized with a number. The effective atomic number depends incident photon energy due to different partial photon interaction processes with material. The effective electron density is called as the numbers of electrons per unit mass. The effective atomic number and electron density give information about the chemical composition of a matter. For instance, if the matter has large effective atomic number, it corresponds to metals or inorganic compound. If the matter has

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small effective atomic number, it corresponds to organic matter. For a long time, the absorption and radiation shielding parameters have been studied on the materials[1-12]. However, these works seem to be limited for the narcotic drugs. Gounhalli et al.[1] calculated the effective atomic numbers and electron densities of few narcotic drugs such as heroin, cocaine, caffeine, tetrahydrocannabinol, cannabinol and tetrahydrocannabivarin from the mass attenuation coefficients for total and partial photon interactions in the energy range 1 keV to 100 GeV using the WinXCOM program.

The aim of this work is provide data for the mass attenuation coefficients, molecular, atomic and electronic cross sections, effective atomic numbers and electron densities of narcotic drugs such as morphine, heroin, cocaine, ecstasy and cannabis. These parameters have been computed for total photon interaction at photon energies from 1 keV to 100 GeV using the WinXCOM program[13].

THEORETICAL BACKGROUND AND COMPUTATION PROCESS

For any complex material, the total mass attenuation coefficient is given as the following equation;

$$\left(\mu/\rho\right)_{comp.} = \sum_i W_i \left(\mu/\rho\right)_i \tag{1}$$

where $(\mu/\rho)_i$ is the total mass attenuation coefficient ith constituent element in the complex material and Wi is the weight fraction of ith constituent element in the complex material. Using the total mass attenuation coefficient values, a number of parameters such as molecular, atomic and electronic cross sections, effective atomic number and electron density can be obtained. The theoretical total mass attenuation coefficient values were then utilized to derive the total molecular cross section and it can be determined as;

$$\sigma_{t,m} = \frac{1}{N}\left(\mu/\rho\right)_{comp.} \sum_i (n_i A_i) \qquad (cm^2 molecule^{-1}) \tag{2}$$

where, N is the Avogadro number, $(\mu/\rho)_{comp.}$ is the total mass attenuation coefficient of complex material, n_i and A_i are the atom number and atomic weight of the ith constituent element in the complex material. Using the total molecular cross section, the total atomic cross section can be obtained simply as following;

$$\sigma_{t,a} = \frac{\sigma_{t,m}}{\sum_i n_i} \qquad (cm^2 atom^{-1}) \tag{3}$$

The total electronic cross section of an element can be computed using the following equation;

$$\sigma_{t,e} = \frac{1}{N}\sum_i \frac{f_i A_i}{Z_i}\left(\mu/\rho\right)_i \qquad (cm^2 electrons^{-1}) \tag{4}$$

where, Z_i is the atomic number of ith element in the complex material and f_i ($f_1+f_2+f_3+....+f_n=1$) is the fractional abundance. The effective atomic number can be derived as follows;

$$Z_{eff} = \frac{\sigma_{t,a}}{\sigma_{t,e}} \tag{5}$$

Finally, the effective electron density or electron number can be determined with the aid of the effective atomic number value;

$$N_E = \frac{Z_{eff}}{A_{tot}}(N n_{tot}) \qquad (electrons g^{-1}) \tag{6}$$

where A_{tot} and n_{tot} are the total atomic weight of complex material and total number of atoms in the complex material. The atomic, molecular and electronic cross sections, effective atomic numbers and electron densities were

computed using the total mass attenuation coefficients which they obtained from the WinXCOM program in the energies from 1 keV to 100 GeV. The WinXCOM program is a Windows version of XCOM[14] based on the mixture rule that gives the attenuation coefficients of any substance as the sum of the appropriately weighted contributions from the individual atoms.

RESULTS AND DISCUSSION

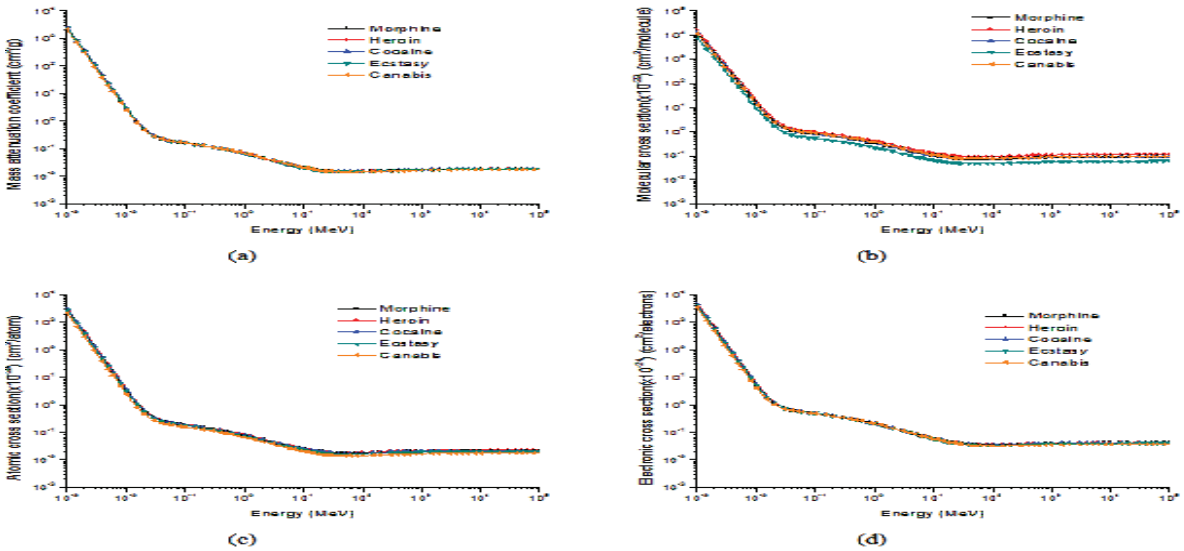
In the present study, the variations of total mass attenuation coefficients, total molecular, atomic and electronic cross sections, effective atomic numbers and electron densities with photon energy for narcotic drugs formed of different elements in different ratios were determined. The molecular formula of selected narcotic drugs is given in Table 1.

TABLE 1. The molecular formula of narcotic drugs

Sample	Morphine	Heroin	Cocaine	Ecstasy	Cannabis
Molecular Formula	$C_{17}H_{19}NO_3$	$C_{21}H_{23}NO_5$	$C_{17}H_{21}NO_4$	$C_{11}H_{15}NO_2$	$C_{21}H_{30}O_2$

The total mass attenuation coefficients, total molecular, atomic and electronic cross sections values were calculated with the help of the Eqs. (1, 2, 3, 4), respectively. The theoretical values of total mass attenuation coefficients, total molecular, atomic and electronic cross sections as a function of photon energy for selected narcotic drugs are given graphically in Fig. 1(a, b, c, d). As seen from Fig. 1, the total mass attenuation coefficient values decrease almost exponentially with increasing photon energy. Besides, the total mass attenuation coefficients decrease with increasing atom number in the narcotic drugs. It is seen from Fig. 1 that there are three energy regions are the predominating attenuation processes. These processes are, low energy towards high energy, photoelectric effect, Compton scattering and pair production, respectively. Since the total mass attenuation coefficient, total molecular, atomic and electronic cross sections have similar tendency, the comments for the total mass attenuation coefficient also valid for the molecular, atomic and electronic cross sections.

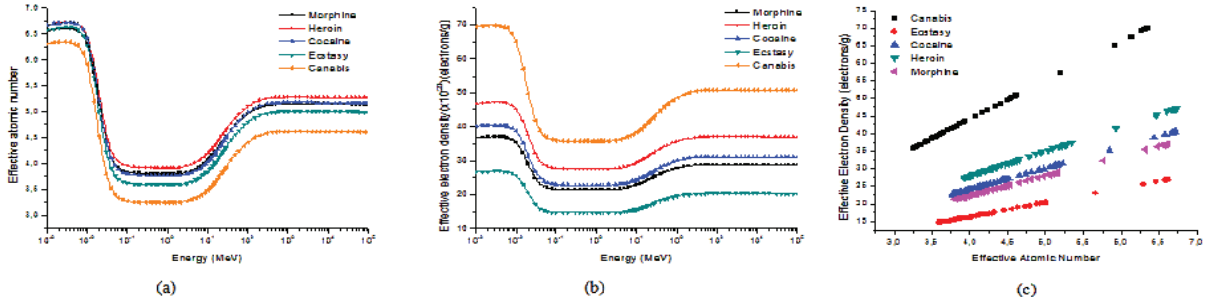
FIGURE 1. Variations of (a) total mass attenuation coefficient (b) molecular cross section (c) atomic cross section (d) electronic cross section versus photon energy



The effective atomic numbers and electron densities values for the present narcotic drugs were computed using the Eqs. (5,6), respectively. The theoretical values of effective atomic numbers and electron densities as a function of photon energy are plotted graphically in the energy range 1 keV to 100 GeV as seen in Fig. 2 (a, b). As seen from Fig. 2, the effective atomic numbers and electron densities of all narcotic drugs are characteristics according to photon energy. It is clearly seen from Fig. 2 that the effective atomic numbers decrease exponentially with increasing photon energy at low energy region. The photoelectric process dominates at low energy region (below

100 keV). The photoelectric effect depends on atomic number as Z^4 for low energy and Z^5 for high energy and the photoelectric effect is inversely proportional with energy as $E^{3.5}$. The minimum values of effective atomic number have been observed in intermediate photon energies (between 0.1-1 MeV) where the Compton scattering process predominates. The Compton scattering depends on atomic number as Z and the Compton scattering is inversely proportional with energy as E. The effective atomic number values are found to be constant in the Compton scattering process. There is a significant variation in effective atomic number values in the high energy region (between 1-300 MeV). In this region, the dominant process is pair production. There is negligible change in effective atomic numbers above 300 MeV energy. The pair production depends on atomic number as Z^2 and the pair production is proportional with energy as E. The behavior of all selected narcotic drugs is almost identical.

FIGURE 2. Variations of (a) effective atomic number (b) electron density versus photon energy (c) effective atomic number versus electron density



As seen from Fig. 2, it is clearly seen that the effective atomic numbers depend on the photon energy, the number of elements in narcotic drugs and the total atomic weight of narcotic drugs. The variations of effective atomic number for selected narcotic drugs with the effective electron density are plotted graphically in Fig. 2 (c). It is clearly seen from this figure, the effective electron density increases linearly with increasing effective atomic number. Since the effective atomic number and electron density have similar tendency, the comments for the effective atomic number also valid for the effective electron density.

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