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Effective Atomic Numbers and Electron Densities of Some HCO Materials as a Function of Weight Fraction of Constituent Elements

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Effective atomic numbers and electron densities of some HCO materials (here HCO materials means organic compounds containing H, C and O only) such as benzyl alcohol, benzaldehyde, ethanol, methanol and glycerol have been computed using computer program over a wide energy range from 1 keV to 100 GeV and the effect of fractional abundance of constituent elements have been investigated and presented in the graphical form.

Key Words: Effective atomic number, Electron density, HCO materials.

INTRODUCTION

Mass attenuation coefficient, effective atomic number and electron density are the basic parameters, which are very useful in determining the interaction of gamma rays through interacting materials. Mass attenuation coefficient measures the number of primary photons which have interactions in the material, effective atomic number is a number assigned to a compound/mixture in a similar way as an atomic number given to elements. However effective atomic number is an energy dependent parameter, which is used to interpret the attenuation of gamma rays through it. Effective electron number or density provides the number of electrons per unit mass of the interacting material.

Mass attenuation coefficient data is now available in the form of software packages WinXCom[1] and XCom[2] for a large number of elements, compounds and mixtures. Further many researchers provide effective atomic numbers[3] in various materials such as alloys[4], amino acids and sugars[5], glasses[6] and semi-conductors[7] at different energies. However electron density data[4-6] is still available only for limited compounds. In the present work, mass attenuation coefficients, effective atomic numbers and electron densities for the selected organic materials over a wide energy range from 1 keV to 100 GeV were computed and finally the effect of weight fraction of the constituent elements was presented in the graphical form.

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COMPUTATIONAL WORK

The mass attenuation coefficients (μ_m) of constituent elements (H, C and O) and the selected organic compounds were obtained from WinXCom computer software. A computer program was prepared to compute molecular cross section (σ_m), atomic cross section (σ_a) and electronic cross section (σ_e), effective atomic number (Z_{eff}) and effective electron number or density (N_{el}) of a compound using the following relations:

$$\sigma_m = (\mu_m)_{comp} \frac{\sum_i n_i A_i}{N} \quad ; \quad \sigma_a = \frac{\sigma_m}{\sum_i n_i} \quad ;$$

$$\sigma_e = \frac{1}{N} \sum_I \frac{f_i A_i}{Z_i} (\mu_m)_i \qquad Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad ; \quad N_{el} = \frac{(\mu_m)_{comp}}{\sigma_e}$$

where N is the Avogadro's number, A_i, f_i, n_i, $(\mu_m)_i$ and Z_i are atomic weight, fractional abundance, number of atoms, mass attenuation coefficient and atomic number of i^{th} element present in a molecule of the organic compound.

RESULTS AND DISCUSSION

In Figs. 1-3, the effect of weight fraction of hydrogen, carbon and oxygen on effective atomic number for some selected incident photon energies have been presented. As shown in Fig. 1, for lower energies *i.e.* upto 10 keV the Z_{eff} have maximum values and shows variable trend with the increase in weight fraction of hydrogen. Initially Z_{eff} values remain constant, thereafter starts increasing, then becomes constant again and finally starts decreasing with the further increase in weight fraction of hydrogen. In the intermediate energy regions *i.e.* from 0.1 to 10 MeV, minimum values have been observed for Z_{eff}, which shows linearly decreasing trend with the increasing weight fraction of hydrogen. For higher energy region *i.e.* above 100 MeV, Z_{eff} values have got intermediate positions *i.e.* their values are less as compare to lower energy region and higher as compare to intermediate energy region.

In Fig. 2, the variation of Z_{eff} values with the weight fraction of carbon shows an opposite trend to that for weight fraction of hydrogen with an exception that Z_{eff} values are maximum in the lower energy region, minimum in the intermediate energy region and in between for the high energy regions. Here the linearly decreasing trend is found in the lower energy region rather than the high-energy region. While at intermediate and high energies varying trends are observed.

Fig. 3. Shows the variation of Z_{eff} with the weight fraction of oxygen. Here, in the lower energy regions, Z_{eff} values increases linearly with the increase in the weight fraction of oxygen, whereas for intermediate and

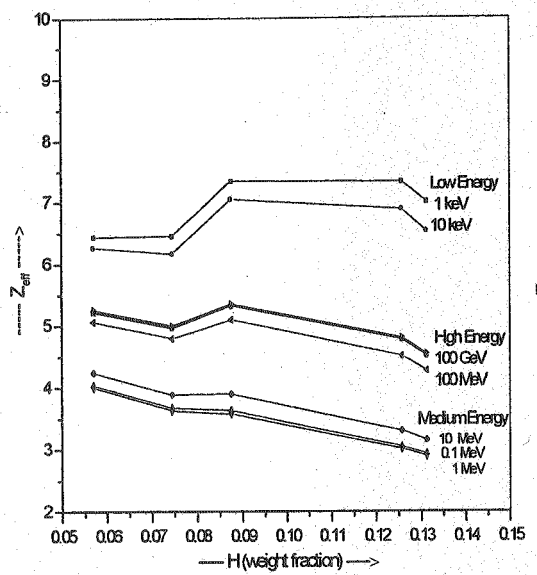

Fig. 1. The variation of effective atomic number with hydrogen weight fraction at some incident photon energies

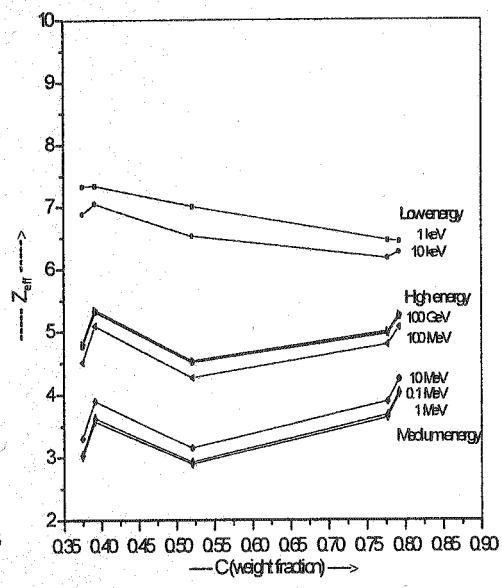

Fig. 2. The variation of effective atomic number with carbon weight fraction at some incident photon energies

high energy regions a similar variable trend is observed. In both intermediate and high-energy regions, Z_{eff} values firstly decreasing slowly, becomes almost constant and then again increases.

Figs. 4-6 shows the variation of the electron density of the selected HCO materials with the weight fractions of the constituent elements at few energies. It is clearly observed in Fig. 4 that for all the energy regions electron density (N_e) increases with the increase in the weight fraction of hydrogen, however the increase is more rapid in the lower energy region than the higher energy region and for the intermediate energy region the rate of increase is the least.

A mixed trend is observed in the variation of electron density with the increase in the weight fraction of carbon and oxygen. For all the energies the trends are same, but the variations are quite sharp in the lower energy region and least for the intermediate energy region, whereas intermediate variation is observed for higher energy region.

Finally, it can be concluded that effective atomic number as well as electron density values behaves differently with the variation of weight fraction of different constituent elements, however values of both parameters are maximum in the lower energy region and minimum in the intermediate energy region and in between for the higher energy region.

Moreover, almost linear relation for all the parameters with the weight fraction of constituent elements in the intermediate energy region confirms the validity of the mixture rule in the intermediate energy region, whereas some experimental studies are still required for the confirmation of the validity of mixture rule in lower as well as higher energy regions.

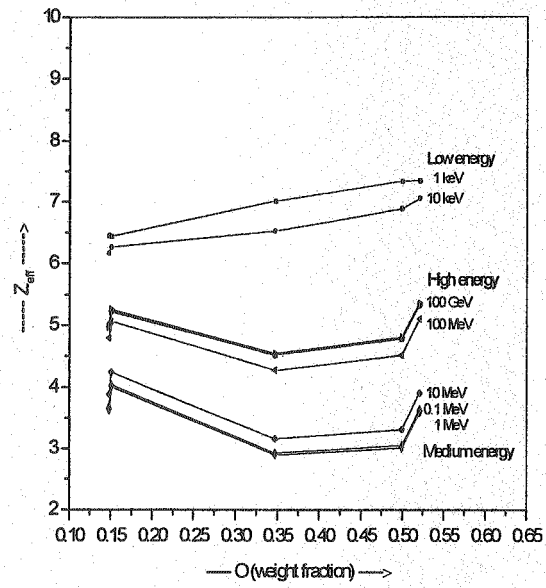

Fig. 3. The variation of effective atomic number with oxygen weight fraction at some incident photon energies.

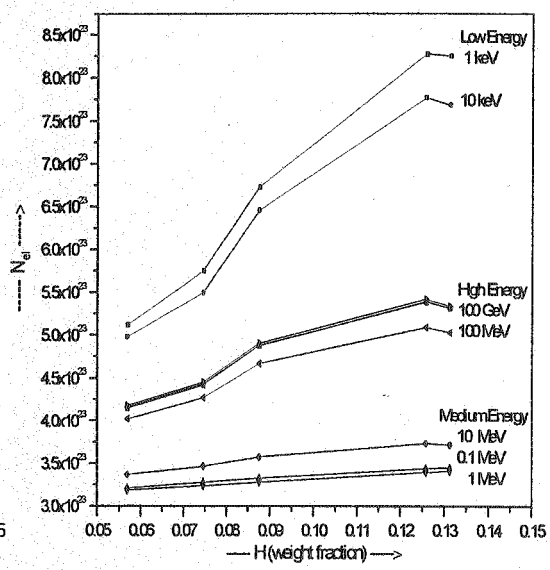

Fig. 4. The variation of electron density with hydrogen weight fraction at some incident photon energies

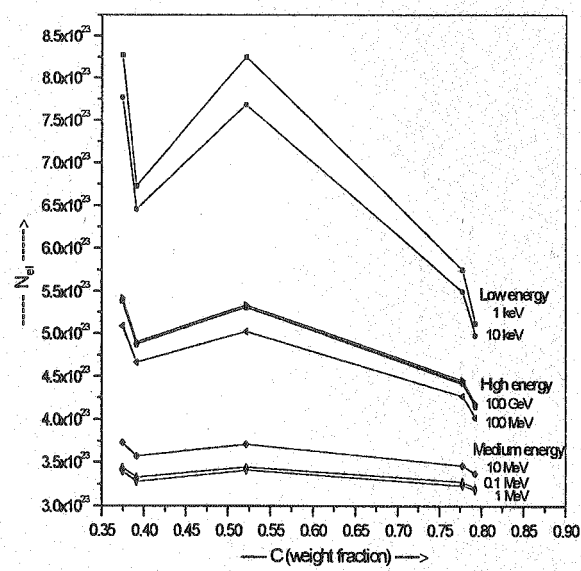

Fig. 5. The variation of electron density with carbon weight fraction at some incident photon energies.

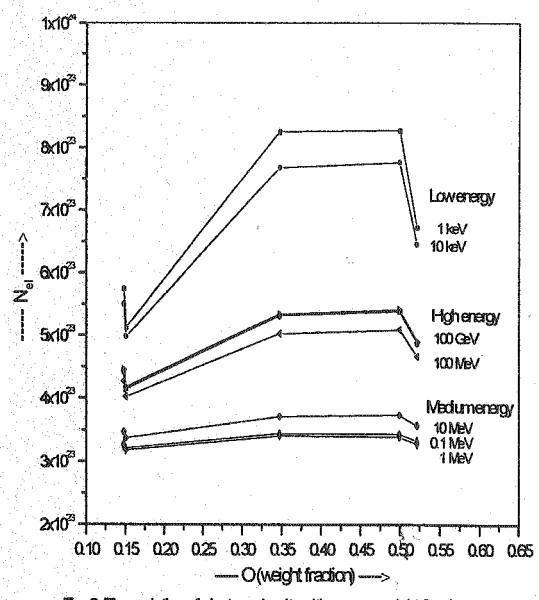

Fig. 6. The variation of electron density with oxygen weight fraction at some incident photon energies.

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