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Study of Photon Interaction with Plasticizers

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Abstract

The effective atomic number and electron density is calculated for some selected Plasticizers like Diethylene glycol dinitrate (DEDGN), Triethylene glycol dinitrate (TEGDN), Butanetriol trinitrate (BTTN), Trimethylolethane trinitrate (TMETN), Diethyl phthalate (DEP) and Diisobutyl phthalate (DIBP) for gamma radiation for energy region 1 keV-100 MeV by using mass attenuation coefficient from WinXCom. It is observed that the values of Z_{eff} and N_{el} changes with energy for different Plasticizers. The variation of effective atomic number with energy for total photon interaction shows the dominance of different interaction process in different energy regions.

Keywords: Mass attenuation coefficients, effective atomic number, effective electron density, plasticizers, energetic materials.

Introduction

The mass attenuation coefficients, effective atomic number and the electron density are the fundamental quantities required in determining the penetration of X-ray, gamma ray and photons in matter. The effective atomic number and the electron density of biological, explosives, energetic materials etc is of significant interest in industrial, biological, agricultural and medical applications. The mass attenuation coefficients give the penetration and deposition of energy in materials.

Plasticizers and super plasticizer are chemical admixtures that can be added to concrete mixtures to meliorate workability. Unless the mix is "starved" of water, the strength of concrete is inversely proportional to the amount of water added. In order to produce stronger concrete, less water is added which makes the concrete mixture less workable and difficult to mix, necessitating the use of plasticizers as a water reducers. Plasticizers are also often used when pozzolanic ash is added to concrete to improve the strength. This method of mix proportioning is especially popular when producing high-strength concrete and fibre-reinforced concrete.

Energetic material pyrotechnic compositions, especially solid rocket propellants and smokeless powders for guns, often employ plasticizers to improve physical properties of the propellant binder or of the overall propellant, to provide a secondary fuel, and ideally, to improve specific energy yield of the propellant. Energetic plasticizers reduce the required mass of propellant, enabling a rocket vehicle to carry more payloads or reach higher velocity. However, safety or cost considerations may demand that non-energetic plasticizers be used, even in rocket propellants. DEP can cause damage to the nervous system as well as to the reproductive organs in males and females[1]. BTTN, TEGDN, TMETN, DEGDN are having applications in solid propellants and also used as an energetic plasticizer in explosives. The plasticizers have wide applications in explosives, propellants and biological field. This has instigated us to carry out this work. The attenuation of gamma and X-ray has motivated lots of researcher to figure out the attenuation coefficients, effective atomic number and electron density. These parameters are determined for alloys[2-4], amino-acids[5-6], thermoluminescent dosimetric (TLD)[7], superconductors[8] and building materials.

Because of diverse applications of γ-radiation, it is very important to know about the processes by which the photons interact with the atoms of the material and get absorbed. Gamma radiations interact with matter predominantly by photoelectric effect, coherent (Rayleigh) and incoherent (Compton) scattering, and pair production process.

In this paper, we estimated the effective atomic number and electron density of selected plasticizers namely, DEDGN ($C_4H_8O_7N_2$), TEGDN ($C_6H_{12}O_8N_2$), BTTN ($C_4H_7O_9N_3$), TMETN ($C_5H_9O_9N_3$), DEP ($C_{12}H_{14}O_4$) and DIBP ($C_{16}H_{22}O_4$) for energy region 1 keV to 100 MeV by using WinXCom[9-10]. The energy dependence of effective atomic number is shown graphically for photon interactions.

Methodology

The method of computation: Effective atomic number and electron density

A parallel beam of mono energetic X-ray or gamma photons passing through matter is attenuated due to absorption and scattering. Attenuation due to absorption follows the Beer–Lambert's law,

$$I = I_o e^{-(\mu/t)x} , \quad (1)$$

Where I_o and I are the intensities of incident and transmitted photon respectively, x is the absorber thickness and μ/ρ is mass attenuation coefficient of the absorbing material.

The mass attenuation coefficient for compound is given by mixture rule[11],

$$(\mu/\rho) = \sum_i w_i \left(\mu/\rho\right)_i \quad (2)$$

w_i and $(\mu/\rho)_i$ are the weight fraction and mass attenuation coefficient of the i^{th} constituting element respectively.

The values of mass attenuation coefficients were then used to determine the total molecular cross-section (σ_m) by the following relation,

$$\sigma_m = \frac{M}{N_A}\left(\frac{\mu}{\rho}\right) \quad (3)$$

Where $M = \sum n_i A_i$ is the molecular weight of the compound, N_A is the Avogadro's number, n_i is the total number of atoms (with respect to mass number) in the molecule, A_i is the atomic weight of the i^{th} element in a molecule.

The effective (average) atomic cross-section (σ_a) can be easily determined from the following equation,

$$\sigma_a = \frac{1}{N_A}\sum f_i A_i \left(\mu/\rho\right)_i \quad (4)$$

Similarly, effective electronic cross-section (σ_e) for the individual element is given by the following formula,

$$\sigma_e = \frac{1}{N_A}\sum \frac{A_i f_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i = \frac{\sigma_a}{Z_{eff}} \quad (5)$$

Where f_i and Z_i are the fractional abundance and atomic number of constituent elements respectively, n_i is the total number of atoms of the constituent element.

Therefore effective atomic number is given as, $Z_{eff} = \frac{\sigma_a}{\sigma_e}$ (6)

The number of electrons per unit mass i.e. effective electron density, N_{el} can be derived by using equations (2) and (5),

$$N_{el} = \frac{N_A}{M} Z_{eff} \sum_i n_i \quad (7)$$

Results and Discussion

In the present study we calculated the Z_{eff} and N_{el} of selected plasticizers namely, DEDGN, TEGDN, BTTN, TMETN, DEP and DIBP for wide range of energy 1 keV to 100 MeV by using WinXCom for partial and total photon interactions. The results are shown graphically in Figures.1-4 for partial and total photon interaction. The calculated values of effective atomic number and effective electron density with respect to photon energy for selected plasticizers are tabulated in tables 1 and 2 for total photon interaction only. The variation of effective atomic number and electron density for photon interactions is discussed in the following paragraphs table-1 and table-2.

Total photon interaction with coherent scattering: The energy dependence of effective atomic number for total photon interaction shows the dominance of different interaction processes in different energy regions as shown in the figure-1. The behaviour of effective atomic number with energy of all plasticizers is almost same. In low energy region, photoelectric interaction is dominant. From figure it is seen that the Z_{eff} decreases rapidly from 8 keV with energy up to 150 keV, it confirms the contribution of scattering process starts dominating due to which it decreases effective atomic number. From 150 keV, the effective atomic number is virtually independent of the energy up to 3 MeV. This is due to the dominance of incoherent scattering in this region. From 3 MeV to 100 MeV, there is regular increase in Z_{eff} with photon energy. This characteristic is due to sharing of incoherent scattering and pair production. It is also observed that the variation of effective atomic number looks upon relative ratio and the range of atomic numbers of the elements of which plasticizers is consists off. The DEDGN, TEGDN, BTTN, and TMETN contain more number of elements when compared with DEP and DIBP. Therefore the change of Z_{eff} with energy is less for compounds which consists of nitrogen. In low energy region, electron density is more for all plasticizers, it's because of the photoelectric interaction is dominant. From 1–8 keV the electron density is almost constant then onwards, there is sharp decrease in N_{el} with energy up to 150 keV, showing that contribution of scattering processes increases which decreases N_{el}. From 150 keV to 3 MeV, N_{el} is almost independent of energy. This may be due to the dominance of incoherent scattering in this region. The N_{el} increases with energy from 3 MeV to 100 MeV it corroborates the dominance of pair production in this region figure-1.

Coherent scattering: The change in Z_{eff} with photon energy for coherent scattering is shown in figure-2. From figure it is observed that effective atomic number increase with the energy in the range 1 keV- 200 keV and remains constant for higher energy for all plasticizers. The Z_{eff} is more for the compounds which consists of nitrogen (DEDGN, TEGDN, BTTN, and TMETN) than the (DEP and DIBP) compounds which doesn't have nitrogen. This is because the contribution is more from nitrogen with the incident energy figure-2.

Table-1
Effective atomic number of selected plasticizers for total photon interaction with coherent

Energy (MeV)	DEDGN	TEDGN	BTTN	TMETN	DEP	DIBP
1E-3	7.48	7.41	7.54	7.48	6.81	6.67
0.0015	7.5	7.43	7.55	7.50	6.84	6.70
0.002	7.52	7.44	7.56	7.51	6.86	6.72
0.003	7.53	7.46	7.57	7.52	6.88	6.73
0.004	7.53	7.46	7.58	7.52	6.88	6.73
0.005	7.52	7.45	7.57	7.52	6.87	6.72
0.006	7.51	7.43	7.56	7.51	6.85	6.69
0.008	7.46	7.37	7.53	7.47	6.76	6.57
0.01	7.38	7.27	7.47	7.40	6.62	6.40
0.015	7.03	6.84	7.21	7.09	6.07	5.75
0.02	6.56	6.30	6.86	6.67	5.46	5.07
0.03	5.77	5.44	6.22	5.95	4.65	4.25
0.04	5.36	5.00	5.85	5.55	4.30	3.91
0.05	5.15	4.79	5.67	5.36	4.15	3.77
0.06	5.05	4.69	5.57	5.26	4.07	3.70
0.08	4.95	4.59	5.48	5.17	4.00	3.63
0.1	4.91	4.56	5.45	5.13	3.97	3.61
0.15	4.88	4.52	5.41	5.10	3.95	3.59
0.2	4.87	4.51	5.40	5.09	3.94	3.58
0.3	4.86	4.51	5.40	5.08	3.94	3.58
0.4	4.86	4.50	5.39	5.08	3.94	3.57
0.5	4.86	4.50	5.39	5.08	3.94	3.57
0.6	4.86	4.50	5.39	5.08	3.93	3.57
0.8	4.86	4.50	5.39	5.08	3.93	3.57
1	4.86	4.50	5.39	5.08	3.93	3.57
1.5	4.86	4.50	5.39	5.08	3.94	3.57
2	4.87	4.51	5.40	5.09	3.94	3.58
3	4.9	4.54	5.43	5.12	3.97	3.60
4	4.94	4.58	5.46	5.15	4.00	3.63
5	4.98	4.62	5.50	5.19	4.03	3.67
6	5.02	4.66	5.54	5.23	4.07	3.70
7	5.06	4.71	5.58	5.27	4.11	3.74
8	5.10	4.75	5.62	5.31	4.14	3.77
9	5.15	4.79	5.65	5.35	4.18	3.81
10	5.18	4.83	5.69	5.39	4.21	3.84
15	5.36	5.02	5.85	5.56	4.37	4.00
20	5.50	5.16	5.97	5.69	4.50	4.13
30	5.71	5.38	6.14	5.88	4.70	4.33
40	5.84	5.53	6.26	6.01	4.83	4.47
50	5.94	5.63	6.34	6.10	4.93	4.57
60	6.01	5.71	6.39	6.16	5.00	4.64
70	6.06	5.77	6.44	6.21	5.06	4.70
80	6.10	5.81	6.47	6.25	5.10	4.75
100	6.16	5.88	6.52	6.30	5.16	4.81

Table-2
Effective electron density of selected plasticizers for total photon interaction with coherent

Energy (MeV)	DEDGN	TEDGN	BTTN	TMETN	DEP	DIBP
1E-3	4.83E23	5.20E23	4.33E23	4.59E23	5.54E23	6.07E23
0.0015	4.84E23	5.22E23	4.34E23	4.60E23	5.56E23	6.09E23
0.002	4.85E23	5.23E23	4.35E23	4.61E23	5.58E23	6.11E23
0.003	4.85E23	5.24E23	4.35E23	4.62E23	5.59E23	6.12E23
0.004	4.85E23	5.24E23	4.35E23	4.62E23	5.59E23	6.12E23
0.005	4.85E23	5.23E23	4.35E23	4.62E23	5.58E23	6.10E23
0.006	4.84E23	5.22E23	4.35E23	4.61E23	5.57E23	6.08E23
0.008	4.81E23	5.18E23	4.33E23	4.58E23	5.50E23	5.97E23
0.01	4.76E23	5.10E23	4.29E23	4.54E23	5.38E23	5.81E23
0.015	4.53E23	4.80E23	4.14E23	4.35E23	4.94E23	5.22E23
0.02	4.23E23	4.42E23	3.94E23	4.09E23	4.44E23	4.61E23
0.03	3.72E23	3.82E23	3.57E23	3.65E23	3.78E23	3.86E23
0.04	3.45E23	3.51E23	3.36E23	3.41E23	3.50E23	3.56E23
0.05	3.32E23	3.37E23	3.25E23	3.29E23	3.37E23	3.42E23
0.06	3.26E23	3.29E23	3.20E23	3.23E23	3.31E23	3.36E23
0.08	3.19E23	3.23E23	3.15E23	3.17E23	3.25E23	3.30E23
0.1	3.17E23	3.20E23	3.13E23	3.15E23	3.23E23	3.28E23
0.15	3.15E23	3.18E23	3.11E23	3.13E23	3.21E23	3.26E23
0.2	3.14E23	3.17E23	3.10E23	3.12E23	3.21E23	3.25E23
0.3	3.14E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
0.4	3.13E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
0.5	3.13E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
0.6	3.13E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
0.8	3.13E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
1	3.13E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
1.5	3.13E23	3.16E23	3.10E23	3.12E23	3.20E23	3.25E23
2	3.14E23	3.17E23	3.10E23	3.12E23	3.21E23	3.25E23
3	3.16E23	3.19E23	3.12E23	3.14E23	3.23E23	3.28E23
4	3.18E23	3.22E23	3.14E23	3.16E23	3.25E23	3.30E23
5	3.21E23	3.24E23	3.16E23	3.19E23	3.28E23	3.33E23
6	3.24E23	3.27E23	3.18E23	3.21E23	3.31E23	3.36E23
7	3.26E23	3.30E23	3.20E23	3.24E23	3.34E23	3.40E23
8	3.29E23	3.33E23	3.23E23	3.26E23	3.37E23	3.43E23
9	3.32E23	3.36E23	3.25E23	3.29E23	3.40E23	3.46E23
10	3.34E23	3.39E23	3.27E23	3.31E23	3.42E23	3.49E23
15	3.46E23	3.52E23	3.36E23	3.41E23	3.55E23	3.63E23
20	3.55E23	3.63E23	3.43E23	3.49E23	3.66E23	3.75E23
30	3.68E23	3.78E23	3.53E23	3.61E23	3.82E23	3.93E23
40	3.77E23	3.88E23	3.60E23	3.69E23	3.93E23	4.06E23
50	3.83E23	3.95E23	3.64E23	3.74E23	4.01E23	4.15E23
60	3.88E23	4.01E23	3.67E23	3.78E23	4.06E23	4.22E23
70	3.91E23	4.05E23	3.70E23	3.81E23	4.11E23	4.27E23
80	3.94E23	4.08E23	3.72E23	3.83E23	4.14E23	4.31E23
100	3.97E23	4.13E23	3.74E23	3.87E23	4.20E23	4.38E23

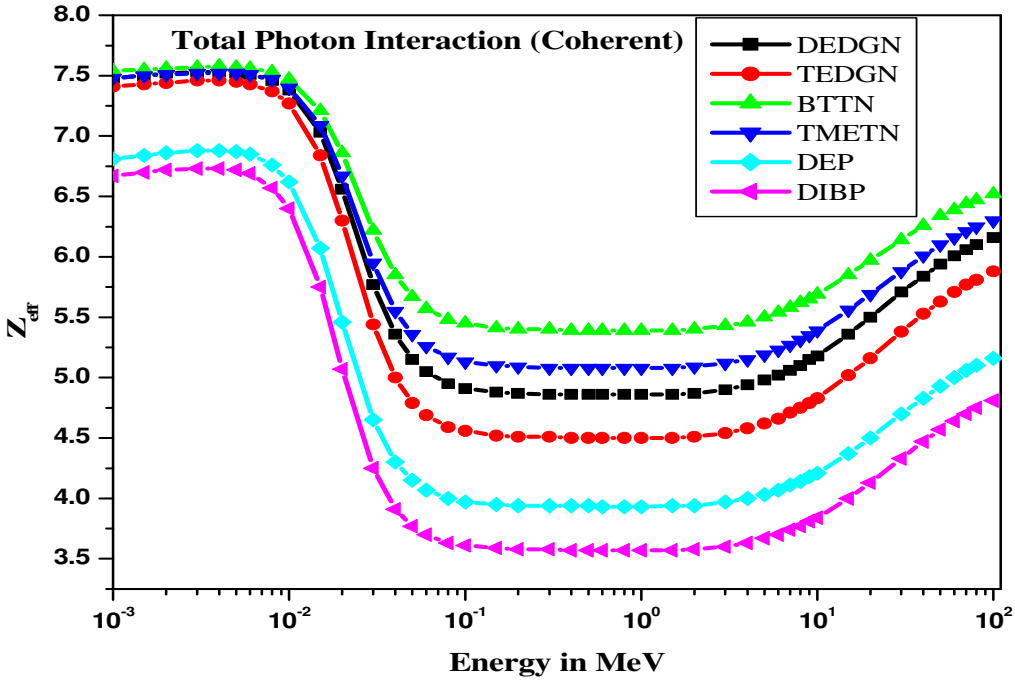

Figure-1
Variation of effective atomic number of selected plasticizers with photon energy for total photon interaction (with coherent)

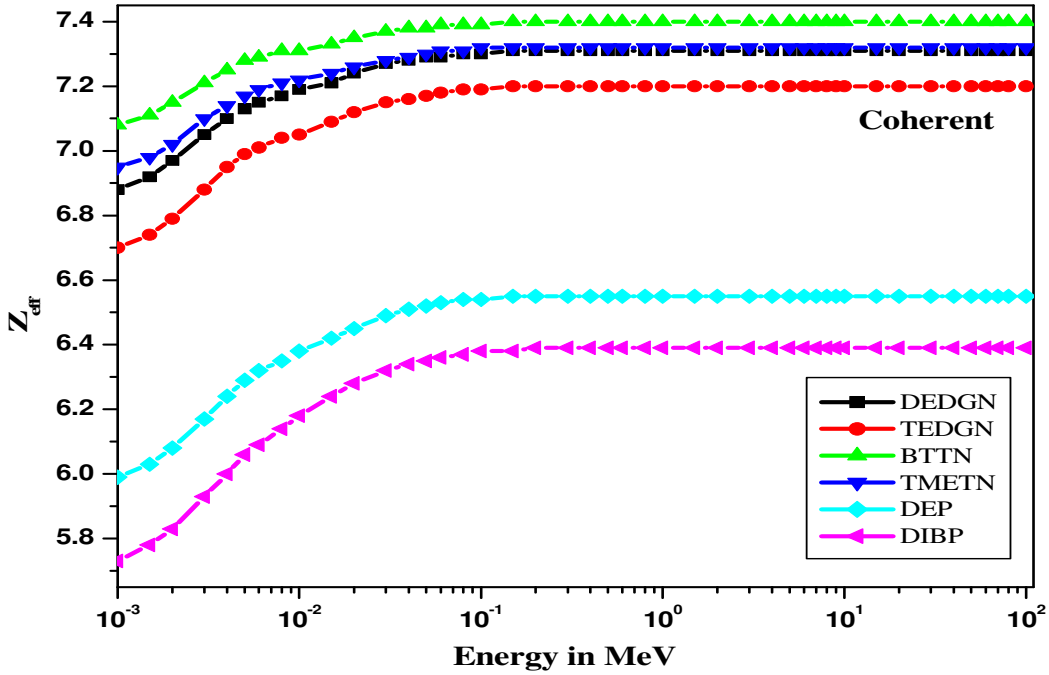

Figure-2
Variation of effective atomic number of selected plasticizers with photon energy for total photon interaction with coherent scattering

Incoherent scattering: The change in effective atomic number with photon energy for incoherent scattering is shown in figure-3, which indicates that Z_{eff} increases acutely with raise in energy up to 200 keV. Above 200 keV, effective atomic number is independent of energy for all plasticizers. Most of the elements in a composite material have a value of

Z/A of about 0.5 where as hydrogen has a value of 1.0, which affects Compton scattering. The present theoretical results are very similar to the Manohara and Hanagodimath[5] and Mudahar et al.[12] who accounted similar types of variations of effective atomic number for amino acids and alloys. The variation of N_{el} with energy is almost same for selected plasticizers figure-3.

Photoelectric absorption: The change in effective atomic number with the energy for photoelectric absorption is shown in figure-4. From figure it is clear that the effective atomic number is increases gradually up to 30 keV and then onwards remains constant with increase in energy figure-4.

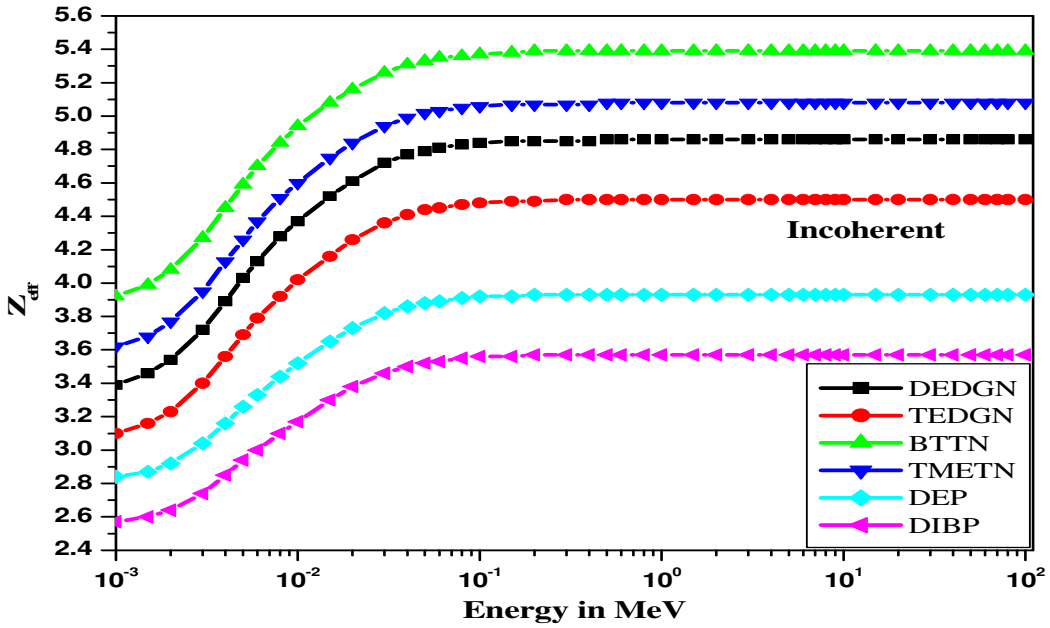

Figure-3

Variation of effective atomic number of selected plasticizers with photon energy for total photon interaction with incoherent scattering

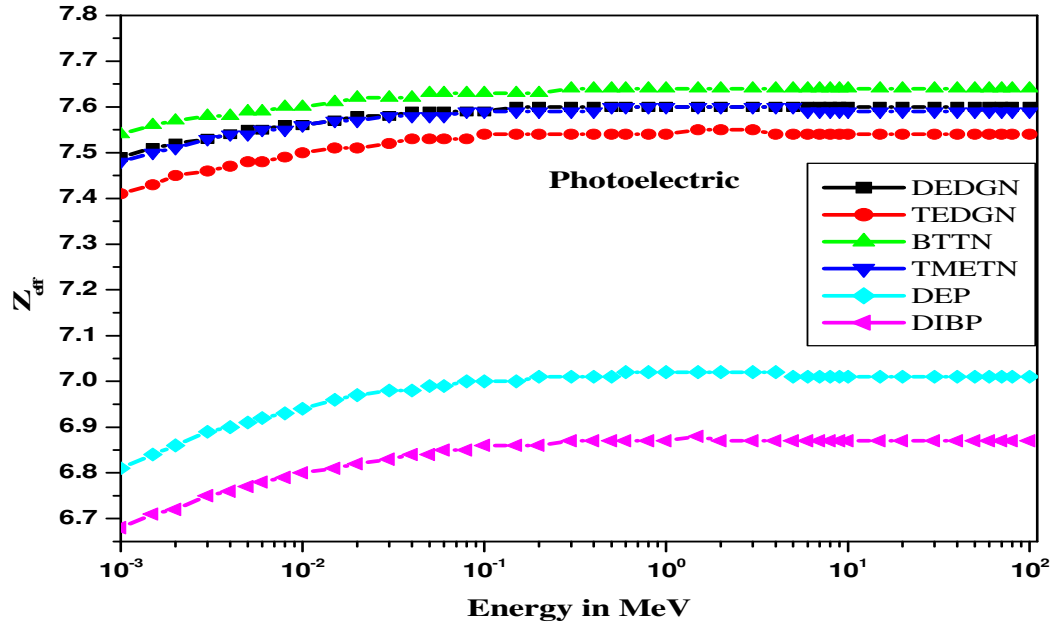

Figure-4

Variation of effective atomic number of selected plasticizers with photon energy for total photon interaction with photoelectric absorption

Conclusion

In the present work we have estimated the change in Z_{eff} and N_{el} with photon energy of selected plasticizers by using WinXCom program. The energy dependence of effective atomic number for total photon interaction shows the potency of different interaction processes in different energy regions. The effective atomic number is nearly constant for the energy region 1 to 8 keV for selected plasticizers and then onwards, it decreases rapidly up to 150 keV, showing that contribution of scattering process increases due to which effective atomic number decreases. From 150 keV to 3 MeV, Z_{eff} is almost independent of energy. This may be due to the dominance of incoherent scattering in this region. From 3 MeV to 100 MeV, the effective atomic number steadily increases with photon energy. This characteristic is due to sharing of incoherent scattering and pair production. It is expected that the new results on Z_{eff} and N_{el} of selected plasticizers presented here will be useful in view of their importance in strengthening the concrete, which will help in the radiation shielding and also in detecting chemical explosives.

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