

Study of mass attenuation coefficients, effective atomic number, electron density and kerma of some coumarin dyes using WinXCom Software

¹Mayadevi Kalgi, ²Shivaleela B, ³Mahantesh B, ⁴JTipperudrappa and ²S M Hanagodimath

¹Department of Physics, Nrupathunga University (Formerly Government Science College), Bangalore-560001, Karnataka, India

²Department of Physics, Gulbarga University, Kalaburagi-585106, Karnataka, India

³Department of Chemistry, P.C. Jabin Science College, Hubli-580031, Karnataka, India

⁴Department of Physics, Vijayanagar Sri Krishnadevaraya University, Ballari-583105, Karnataka, India

mayavnn1@gmail.com, shivaleelbphysics@gmail.com, mahanteshachem@gmail.com,
jtrphy2007@gmail.com, smhmth@gmail.com,

Abstract—The effective atomic number (Z_{eff}) and electron density (N_{el}) of coumarin derivatives 1IPBC and 4IP6MC have been calculated for all photon interactions [coherent, incoherent, photoelectric, pair production in the field of electric and nuclear, total photon interaction (with coherent and incoherent)] in the energy range 1 keV to 100 GeV using the WinXCom program. The significant variation of photon mass attenuation coefficient, Z_{eff} and N_{el} is due to the variations in the dominance of different interaction processes in different energy regions. The maximum values of Z_{eff} and N_{el} are found in the low-energy range ($E > 0.5$ MeV), where photoelectric absorption is the main interaction process for total photon interaction (with coherent). The minimum values of Z_{eff} and N_{el} are found at intermediate energies, typically $2 \text{ MeV} < E < 400 \text{ MeV}$, where Compton scattering is dominant. Above 400 MeV, Z_{eff} and N_{el} assume an almost constant value determined by pair production. The Kerma (K_a) values also have been calculated for energy range 1 keV–20 MeV. It is to be noted that K_a values show sharp peak due to photoelectric absorption of the high-Z constituent of the compound.

Index Terms—Coumarin dyes, mass attenuation coefficient, effective atomic number, electron density, WinXCom

I. INTRODUCTION

Coumarin and its derivatives have potential application in various fields of science and technology [1-4]. They create a family of dyes, which have uses in physics, chemistry, biology and medicine [5]. They have a strong UV-visible fluorescence, making them excellent for usage as colorants, dye laser media and nonlinear optical chromophores [6, 7]. These diverse compounds are extensively used in areas as food preservatives, cosmetics fluorescent indicators and insecticides. They have attracted significant interest in pharmaceutical research areas such as antiviral, anticancer, anti-inflammatory, hepatoprotective, anticarcinogenic and anticoagulant activities [8-14]. It is observed from literature that 4-aryloxymethyl coumarins exhibited antimicrobial activity, long range coupling and centrosymmetric nature. Novel dyes 1-(2-iodo phenoxy methyl)-benzo[f]chromen-3-one (1IPBC) and 4-aryloxymethyl coumarin 4-(2-iodo phenoxy methyl)-6-methoxychromen-2-one (4IP6MC) exhibited better anti-cancer and antimicrobial activities. We have selected these coumarin dyes in studying the effective atomic number and electron density parameters.

The photon has begun to be used in a variety of industries, including medicine, agriculture, aviation, and power plants after development of technology [15]. The essential quantities necessary in determining the penetration of X-rays/gamma photons in matter are mass attenuation coefficients (μ/ρ), effective atomic number (Z_{eff}), and electron density (N_{el}) [16]. In primary physics and several applied fields, mass attenuation is a special feature. The mass attenuation coefficient is a measurement of how strongly a substance absorbs or scatters light per unit mass per unit area at a certain wavelength [17]. At the same photon energy, mass attenuation coefficients tend to rise with increasing atomic number, so materials used to shield X-ray and gamma radiation have large atomic numbers (with high mass attenuation coefficients). Precise measurements of X-ray and γ -ray mass attenuation coefficients in material are required in a variety of applications, including nuclear diagnostics, radiation protection, nuclear medicine, and radiation dosimetry [18].

For the first time, Hine [19] proposed the idea of effective atomic number for compounds and mixtures. The effective atomic number of a substance made up of numerous elements, according to Hine, cannot be described by a single number and the various atomic numbers in the material must be weighed differently for each of the various ways by which γ -rays could interact with matter. The "effective atomic number" is a number that changes with the energy of compounds and mixes. Considering Hine's advice, many attempts have been made to establish effective atomic number (Z_{eff}) for different materials. The effective electron density (N_{el}) of composite materials is the number of effective electrons per unit mass, which may be calculated using Z_{eff} [20]. The most popular way for estimating Z_{eff} and N_{el} values has been proven to be the atomic or electronic cross-section approach.

In the present work, results computed on the mass attenuation coefficient, effective atomic numbers and electron densities for selected organic molecules in the broad energy range from 1 keV to 100 GeV using WinXCOM. The kerma relative to air has been calculated in the energy range 0.001–20 MeV. The aim of this work is to investigate interaction of gamma rays with coumarin molecules in this wide energy range and also the significant variation of Z_{eff} and N_{el} with energies for total and partial photon interactions like coherent, incoherent, photoelectric, pair production in electric and nuclear field.

II. COMPUTATIONAL METHODS

The mass attenuation coefficients of the coumarins 1IPBC and 4IP6MC were determined using mixing rule and the WinXcom programme introduced by Gerward[21, 22]. It can provide an interface that enables defining, editing, and saving substances in a substance definition list easier. For the conventional energy range (1 keV–100 GeV), a user-selected energy, or a combination of the two, WinXCom can calculate cross sections and attenuation coefficients. The WinXCom code can also be used to determine the cross-section or attenuation coefficient as a function of the photons' energy using total gamma photon interaction, a valid method was utilised to calculate the effective atomic numbers and electron densities of coumarins[23]. In the energy range 1 keV–20 MeV, Kerma relative to air has also been determined using the applicable formula. Because the variation is insignificant, the effect on the outcomes will be negligible [24].

III. THEORETICAL BACKGROUND

Using the WinXCom and the subsequent "mixing rule," the total photon mass attenuation coefficient $(\mu/\rho)_{comp}$ for a chemical compound or mixture was computed.

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

where $(\mu/\rho)_i$ and ω_i are the photon mass attenuation coefficient and the weight fraction of the i th constituent element in the compound, respectively. The quantity ω_i of a material made up of multiple constituents is given by[25]

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

With condition that

$$\omega_1 + \omega_2 + \omega_3 + \omega_4 + \dots = 1$$

where A_i is the i th element's atomic weight and n_i is the number of formula units in the element.

The effective molecular cross section (σ_m) is estimated using the values of mass attenuation coefficients $(\mu/\rho)_{comp}$ by the following relation

$$\sigma_m = \left(\frac{\mu}{\rho}\right)_{comp} \frac{\sum_i n_i A_i}{N} \quad (3)$$

where N is the Avogadro's number, n_i and A_i are the total number of atoms and atomic weight of the i th element in a molecule respectively[26].

The total cross section (σ) and different partial cross-sections[17] are related by the relation

$$\sigma = \sigma_{coh} + \sigma_{incoh} + \tau + \kappa + \sigma_{ph,n} \quad (4)$$

Where σ_{coh} and σ_{incoh} are the scattering cross-sections of coherent and incoherent processes, respectively. τ is the atomic photoelectric cross-section, $\sigma_{ph,n}$ is the photonuclear cross-section, and κ is the positron electron pair production cross-section.

The following equation connects the effective atomic cross-section (σ_a) and the effective molecular cross-section (σ_m),

$$\sigma_a = \frac{\sigma_m}{\sum_i n_i} \quad (5)$$

Similarly, electronic cross-section (σ_e) is given by the following equation[27,28]:

$$\sigma_e = \frac{1}{N} \sum_i \left(\frac{f_i A_i}{Z_i} \right) \left(\frac{\mu}{\rho} \right)_i \quad (6)$$

where A_i and $f_i = n_i / \sum_i n_i$ are the atomic number and fractional abundance of the constituent element.

Effective atomic number (Z_{eff}) is the ratio of the atomic and electronic cross-sections and it is given by[29]

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad (7)$$

Using the above equations Manohara et al [26] have shown that Z_{eff} is given by

$$Z_{eff} = \frac{\sum_i n_i A_i \left(\frac{\mu}{\rho} \right)_i}{\sum_i n_i \frac{A_i}{Z_i} \left(\frac{\mu}{\rho} \right)_i} \quad (8)$$

here Z_i is the atomic number of the i th element present in a molecule. The effective electron density (N_{el}) which is another parameter related to Z_{eff} , which represents the number of electrons per unit mass of interacting materials and may be computed using the following relationship[30, 31],

$$N_{el} = \frac{(\mu/\rho)_{comp} Z_{eff}}{\sigma_a} \quad (9)$$

Kerma is an acronym for "kinetic energy released per unit mass", defined as the sum of the initial kinetic energies of all the charged particles liberated by uncharged ionizing radiation in a sample of matter, divided by the mass of the sample. This quantity, $\text{J kg}^{-1} = \text{Gy}$, is applicable to both photons (x-ray, gamma, bremsstrahlung, etc.) and neutrons as the absorbed dosage. In order to compute the Kerma relative to air μ_{en}/ρ -absorption coefficient[32], and Coumarin derivatives were calculated using the equation (10)

$$K_a = \frac{(\mu_{en}/\rho)_{comp}}{(\mu_{en}/\rho)_{air}} \quad (10)$$

IV. RESULTS AND DISCUSSION

Mass attenuation coefficients

The molecular formula of coumarin derivatives is presented 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. Photoelectric absorption, Compton scattering and pair production are the three dominant attenuation mechanisms, as shown in the graph. Mass attenuation coefficient values varies significantly below 100 keV and considerably between 150 keV and 40 MeV, with negligible variation above 40 MeV photon energy[33-36]. In low energy region photoelectric absorption is dominant, in intermediate energy range Compton scattering is dominant and, in high energy range pair production is dominant interaction process.

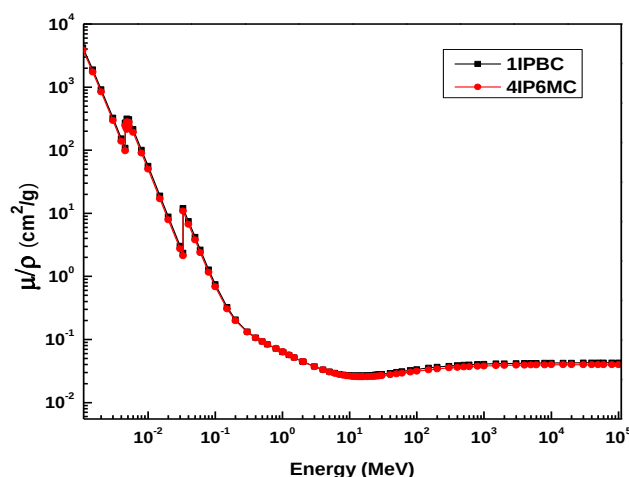


Fig. 1: Variation of photon mass attenuation coefficient $(\mu/\rho)_c$ of coumarin dyes with photon energy for total photon interaction (with coherent).

Table 1. Name of the compound with molecular formula.

S. No.	Name of the compound	Molecular formula
1	1IPBC	C ₁₅ H ₁₁ O ₄ I
2	4IP6MC	C ₂₀ H ₁₃ O ₃ I

Effective atomic number and electron density

The calculation of Z_{eff} and N_{el} of coumarin dyes 1IPBC and 4IP6MC were carried out using cross sectional data which were exported to MS Excel from WinXCom. These data shows that both the parameters depend upon chemical composition of the given molecule or compound. The Z_{eff} and N_{el} values of coumarin dyes for varying energies have been given in Table 2 for all photon interaction processes in the energy region 1 keV-100 GeV and also variation shown graphically.

a) Total photon interaction (with coherent and incoherent)

The Z_{eff} and N_{el} are mainly dominated by different partial photon interaction processes, it can be easily seen from Fig. 2 (a & b) that in the continuous energy range (1 keV– 100 GeV). Energy below 0.5 MeV, Z_{eff} has maximum values, where photoelectric interaction is dominant. Z_{eff} drops to a lower value typically for Compton scattering, in the energy region 0.5-2 MeV. Compton scattering or incoherent scattering is the main interaction process between 2-40 MeV energy region in this intermediate energy

range and Z_{eff} is about constant and equal to mean (average) atomic number [37, 38]. Z_{eff} rises with increasing energy in the 40–400 MeV transition zone as pair production progressively takes over. At high energies above 400 MeV, Z_{eff} assumes an almost constant value determined by pair production.

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 the coumarin derivatives, then 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. 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 creation.

As a result of the above, the photoelectric absorption cross-section, which is proportional to Z^4-5 , gives larger weight to the high Z elements than the other processes. The greatest values of Z_{eff} in the low energy zone are readily explained by this state. In contrast to photoelectric absorption and pair production processes, the Compton scattering cross-section is proportional to Z, giving high Z elements less weight [39].

Electron density is closely related to the effective atomic number, as shown by Equation (3). As a result, N_{el} qualitative energy dependence is similar to Z_{eff} . The total incoherent processes for 4IP6BC compound observed slight higher N_{el} values than 1IPBC, can be seen in Fig. 2 (b). Furthermore, within the dominance region of any of the three major photon interaction processes, the effective atomic number values remain constant, but the values of effective atomic number vary in the regions where the dominance region for one process shifts to the other. The presence of absorption edges of the constituent parts creates an exception in the lower energy zone [20].

b) Coherent and incoherent scattering

The Z_{eff} variation for coherent scattering with photon energy is shown in Fig. 2 (c & d). It is apparent from the figures that Z_{eff} increases as energy increases from 1 keV to 4 keV. It decreases abruptly around 5 keV from 4 keV, then gradually rises to 1 MeV. Beyond that extent, Z_{eff} remains constant as energy is increased. Because of the inclusion of phosphorus, the behaviour differs from that of other organic molecules [40]. It has demonstrated that in materials comprising carbon, hydrogen, and oxygen, the effective atomic numbers tend to be constant as a function of energy. Similarly, the variation of Z_{eff} with photon energy for incoherent scattering is shown in Fig. 2 (d) which indicates that Z_{eff} increases sharply in energy in the region 1 keV–100 GeV.

d) Pair production in nuclear field and electric field

Pair production in the nuclear field, the change of Z_{eff} with photon energy is shown in Fig. 2 (e), which demonstrates that Z_{eff} increases significantly with increasing photon energy from 10 to 26 MeV before becoming almost energy independent [41]. It could be because pair production in the nuclear field is Z_2 dependent. Due to the inclusion of elements with a wide range of atomic numbers, the increase in Z_{eff} with energy is more significant in 1IP6MBC below 10 MeV than in 4IP6MC. Z_{eff} is independent of photon energy from 26 keV to 50 GeV, as shown in the figure. From 50 GeV, Z_{eff} increases with increasing photon energies up and then it is independent of energy thereafter for both the compounds. Similarly, the variation of Z_{eff} with photon energy for electric field is shown in Fig. 2 (f). The variation is nearly same for 1IPBC and 4IP6MC.

e) Photoelectric absorption

A plot of Z_{eff} vs photon energy, especially for medium and high-Z materials, shows the distinctive absorption edges as the binding energy of each electron subshell is reached and a new pathway for photoexcitation is energetically enabled [17]. Fig 2 (g) demonstrate the fluctuation of Z_{eff} with photon energy for photoelectric absorption, indicating that Z_{eff} is nearly independent of photon energy. This is due to the fact that these biological substances are made up of elements with the same or similar atomic numbers. Z_{eff} increases sharply from 1 keV to 8 keV and then it remains almost constant thereafter. This is because, photoelectric process is predominant at low energies (1 MeV) and for materials of higher atomic numbers [42].

The variations of N_{el} with photon energy in all the biological compounds for partial and total interaction processes are similar to that of Z_{eff} shown in Figs. 3 (a-g) and can be explained on a similar manner as that of Z_{eff} . This is also evident from the fact that both molecules have a mean atomic number $\langle Z \rangle$, for total photon interaction process, of about 27.35. The average value of electron density $\langle N_{\text{el}} \rangle$, have been calculated and it is about 13.35. The average values for different process also has been given in Table 3. The values of $\langle Z_{\text{eff}} \rangle$ and $\langle N_{\text{el}} \rangle$ are maximum for Photoelectric absorption and coherent processes than other photon interaction processes.

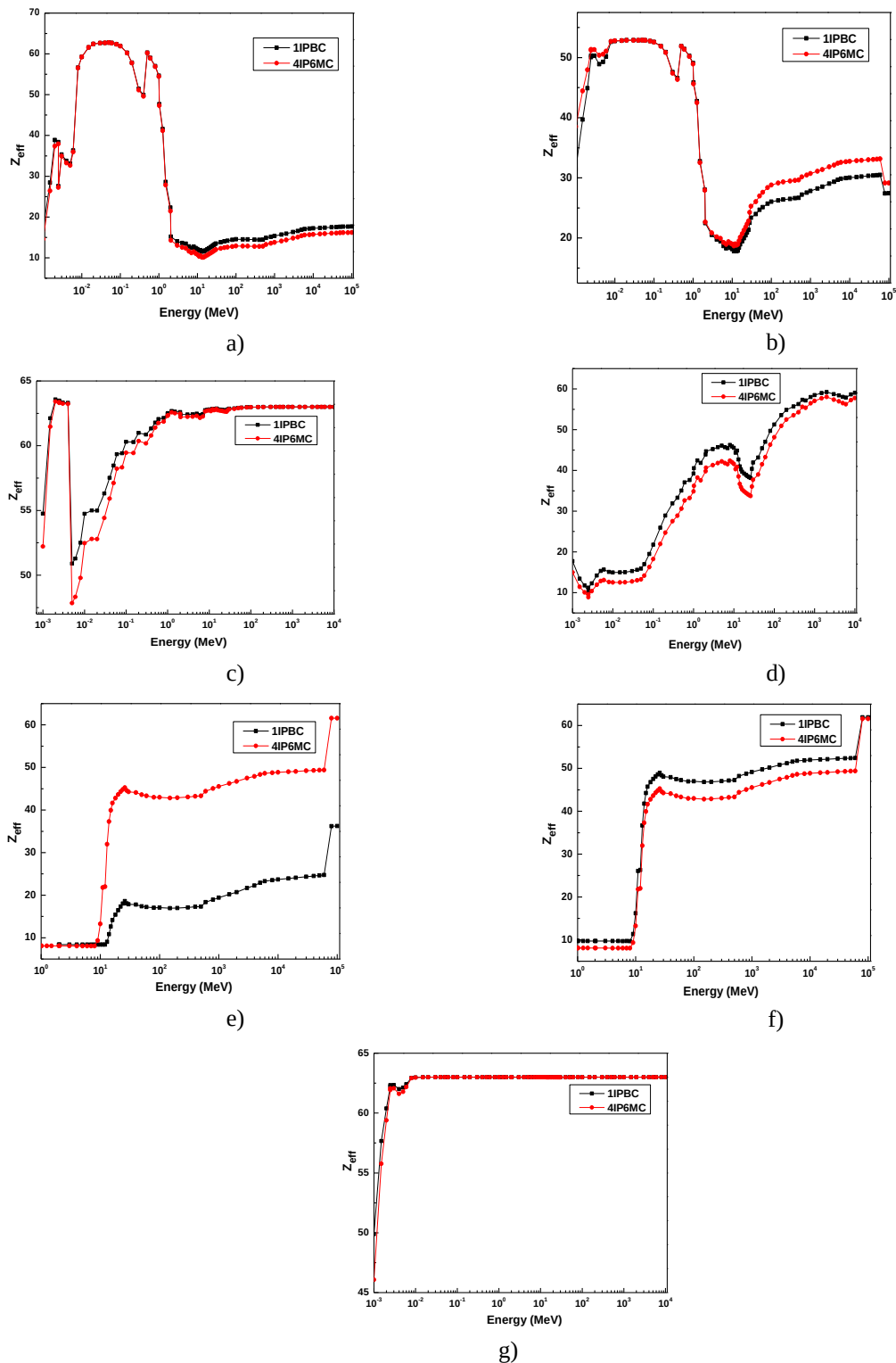


Fig. 2. Energy dependence of the effective atomic number Z_{eff} , of Coumarin dyes for (a) total photon interaction (with coherent) (b) total photon interaction (with incoherent). (c) coherent (d) incoherent (e) pair nuclear (f) pair electron (g) photoelectric absorption.

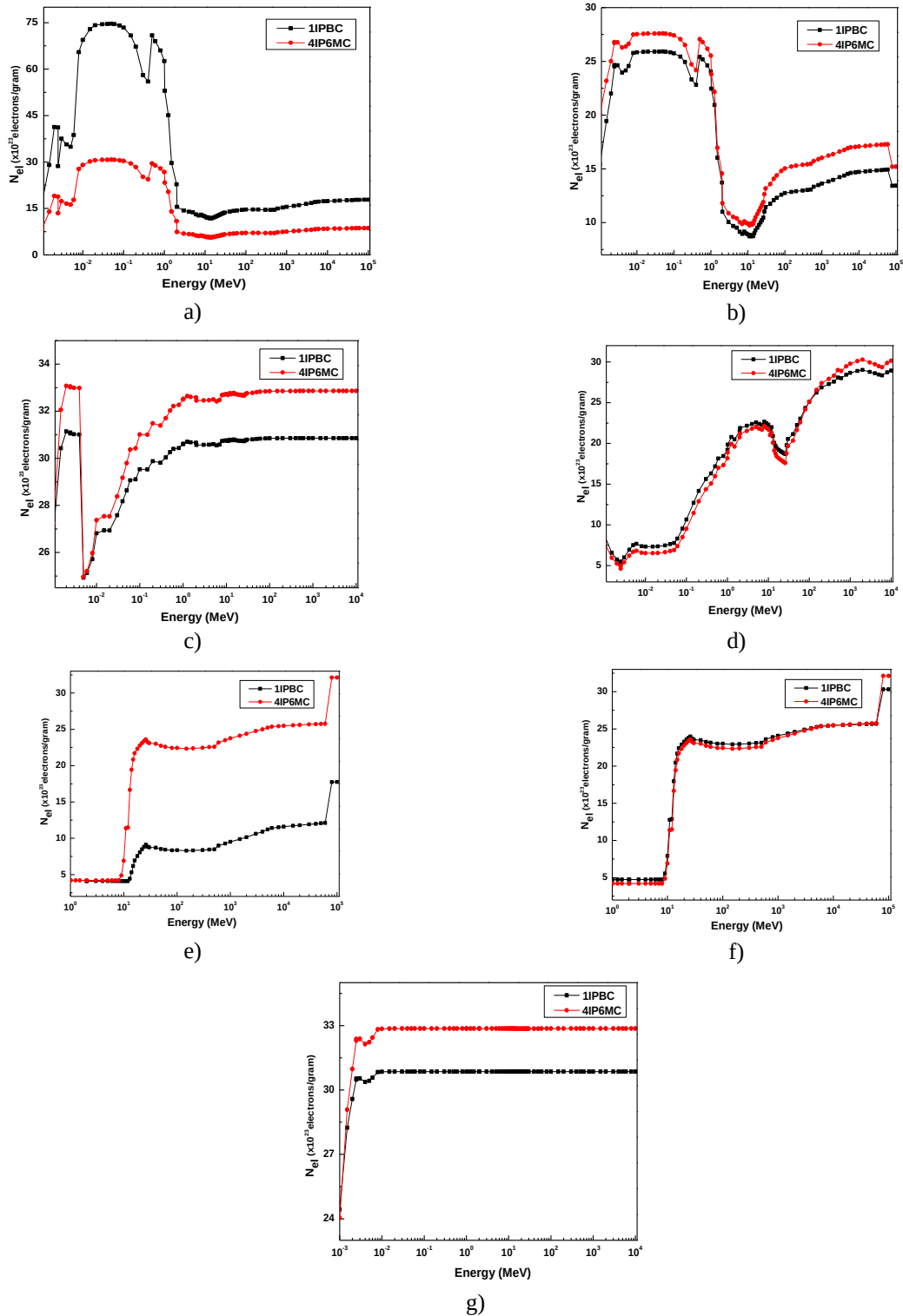


Fig.3. Energy dependence of the electron density $N_{eI}(10^{23}\text{electrons/gram})$, of Coumarin dyes for (a) total photon interaction (with coherent) (b) total photon interaction (with incoherent). (c) coherent (d) incoherent (e) pair nuclear (f) pair electron (g) photoelectric absorption.

Table 2 Effective atomic number and electron densities (*10²³electrons/gm) of fluorescent compounds for total photon interaction (with coherent) in the energy range of 1 keV-100 GeV.

Energy (MeV)	1IPBC				4IP6MC			
	Z _{eff}		N _{el}		Z _{eff}		N _{el}	
	Tot Coh	Tot Incoh	Tot Coh	Tot Incoh	Tot Coh	Tot Incoh	Tot Coh	Tot Incoh
1.00E-03	31.45	17.11	15.41	8.38	38.51	14.23	20.09	7.42
1.50E-03	39.70	28.46	19.44	13.94	44.46	24.38	23.19	12.72
2.00E-03	44.92	38.86	22.00	19.03	47.95	34.66	25.01	18.08
2.47E-03	50.08	38.36	24.53	18.79	51.22	34.54	26.72	18.02
2.47E-03	50.34	27.54	24.66	13.49	51.36	24.08	26.79	12.56
3.00E-03	50.29	35.33	24.63	17.30	51.31	31.52	26.76	16.44
4.00E-03	48.90	33.79	23.95	16.55	50.38	29.94	26.28	15.62
5.00E-03	49.29	33.12	24.14	16.22	50.56	29.31	26.37	15.29
6.00E-03	50.15	36.32	24.57	17.79	51.05	32.51	26.63	16.96
8.00E-03	52.62	56.62	25.77	27.73	52.70	54.99	27.49	28.69
1.00E-02	52.75	59.29	25.84	29.04	52.78	58.28	27.53	30.40
1.50E-02	52.82	61.60	25.87	30.17	52.83	61.19	27.56	31.92
2.00E-02	52.88	62.42	25.90	30.58	52.88	62.25	27.59	32.47
3.00E-02	52.89	62.65	25.90	30.69	52.88	62.54	27.59	32.62
4.00E-02	52.88	62.69	25.90	30.70	52.87	62.59	27.58	32.65
5.00E-02	52.90	62.75	25.91	30.74	52.90	62.68	27.59	32.70
6.00E-02	52.87	62.67	25.89	30.70	52.86	62.57	27.57	32.64
8.00E-02	52.75	62.36	25.84	30.55	52.73	62.17	27.51	32.43
1.00E-01	52.58	61.93	25.75	30.33	52.56	61.62	27.42	32.14
1.50E-01	51.92	60.28	25.43	29.52	51.88	59.50	27.06	31.04
2.00E-01	50.92	57.85	24.94	28.34	50.83	56.47	26.52	29.46
3.00E-01	47.59	51.39	23.31	25.17	47.40	48.73	24.73	25.42
4.00E-01	46.56	49.89	22.81	24.44	46.35	47.00	24.18	24.52
5.00E-01	51.91	60.29	25.43	29.53	51.87	59.52	27.06	31.05
6.00E-01	51.43	59.03	25.19	28.91	51.37	57.93	26.79	30.22
8.00E-01	50.27	57.00	24.62	27.92	50.17	55.42	26.17	28.91
1.00E+00	49.08	54.64	24.04	26.76	48.94	52.55	25.53	27.41
1.02E+00	45.84	47.66	22.46	23.34	45.62	44.48	23.80	23.20
1.25E+00	42.76	41.57	20.94	20.36	42.49	37.86	22.16	19.75
1.50E+00	32.75	28.60	16.04	14.01	32.52	24.91	16.96	12.99
2.00E+00	28.02	22.29	13.72	10.92	27.93	19.15	14.57	9.99
2.04E+00	22.47	15.17	11.01	7.43	22.64	13.02	11.81	6.79
3.00E+00	20.52	14.03	10.05	6.87	20.84	12.05	10.87	6.28
4.00E+00	19.76	13.63	9.68	6.68	20.17	11.70	10.52	6.10
5.00E+00	19.44	13.45	9.52	6.59	19.92	11.53	10.39	6.02
6.00E+00	18.67	12.79	9.14	6.26	19.25	10.97	10.04	5.72
7.00E+00	18.28	12.42	8.95	6.09	18.94	10.66	9.88	5.56
8.00E+00	18.69	12.73	9.15	6.23	19.38	10.91	10.11	5.69
9.00E+00	18.36	12.37	8.99	6.06	19.12	10.61	9.97	5.53
1.00E+01	18.16	12.12	8.89	5.94	18.98	10.39	9.90	5.42
1.10E+01	17.79	11.72	8.71	5.74	18.69	10.06	9.75	5.25
1.20E+01	18.07	11.86	8.85	5.81	19.01	10.18	9.91	5.31

1.30E+01	17.80	11.54	8.72	5.65	18.80	9.91	9.81	5.17
1.40E+01	17.90	11.53	8.77	5.65	18.95	9.90	9.88	5.16
1.50E+01	18.40	11.64	9.01	5.70	19.52	9.98	10.18	5.21
1.60E+01	18.92	11.79	9.27	5.78	20.11	10.11	10.49	5.28
1.80E+01	19.45	12.08	9.53	5.92	20.70	10.34	10.80	5.40
2.00E+01	19.96	12.36	9.78	6.05	21.27	10.56	11.09	5.51
2.20E+01	20.45	12.61	10.02	6.18	21.81	10.77	11.38	5.62
2.40E+01	20.91	12.86	10.24	6.30	22.33	10.96	11.65	5.72
2.60E+01	21.34	13.08	10.45	6.41	22.81	11.15	11.90	5.81
2.80E+01	22.53	13.29	11.03	6.51	24.25	11.31	12.65	5.90
3.00E+01	23.35	13.50	11.44	6.61	25.27	11.48	13.18	5.99
4.00E+01	23.97	13.83	11.74	6.77	26.04	11.74	13.58	6.13
5.00E+01	24.68	14.05	12.09	6.88	26.98	11.91	14.07	6.22
6.00E+01	25.12	14.19	12.31	6.95	27.58	12.03	14.39	6.27
8.00E+01	25.70	14.40	12.59	7.05	28.39	12.19	14.81	6.36
1.00E+02	26.02	14.54	12.75	7.12	28.82	12.30	15.03	6.42
1.50E+02	26.24	14.53	12.85	7.12	29.14	12.29	15.20	6.41
2.00E+02	26.38	14.53	12.92	7.12	29.32	12.29	15.30	6.41
3.00E+02	26.50	14.43	12.98	7.07	29.46	12.22	15.37	6.37
4.00E+02	26.61	14.41	13.03	7.06	29.58	12.20	15.43	6.37
5.00E+02	26.68	14.44	13.07	7.07	29.65	12.23	15.47	6.38
6.00E+02	27.21	14.87	13.33	7.28	30.15	12.58	15.73	6.56
8.00E+02	27.54	15.14	13.49	7.42	30.47	12.82	15.89	6.69
1.00E+03	27.82	15.36	13.63	7.53	30.72	13.00	16.03	6.78
1.50E+03	28.23	15.68	13.83	7.68	31.11	13.27	16.23	6.92
2.00E+03	28.53	15.92	13.97	7.80	31.37	13.47	16.37	7.03
3.00E+03	29.04	16.32	14.22	8.00	31.84	13.82	16.61	7.21
4.00E+03	29.33	16.57	14.37	8.12	32.11	14.03	16.75	7.32
5.00E+03	29.66	16.88	14.53	8.27	32.41	14.30	16.91	7.46
6.00E+03	29.85	17.06	14.62	8.35	32.58	14.45	16.99	7.54
8.00E+03	29.95	17.15	14.67	8.40	32.67	14.53	17.04	7.58
1.00E+04	30.03	17.23	14.71	8.44	32.74	14.59	17.08	7.61
1.50E+04	30.14	17.32	14.76	8.48	32.84	14.67	17.13	7.65
2.00E+04	30.21	17.38	14.80	8.52	32.90	14.73	17.16	7.68
3.00E+04	30.32	17.48	14.85	8.56	33.01	14.81	17.22	7.73
4.00E+04	30.38	17.54	14.88	8.59	33.06	14.86	17.25	7.75
5.00E+04	30.44	17.60	14.91	8.62	33.12	14.91	17.27	7.78
6.00E+04	30.48	17.63	14.93	8.64	33.15	14.94	17.29	7.79
8.00E+04	27.42	17.65	13.43	8.65	29.13	14.96	15.20	7.80
1.00E+05	27.43	17.66	13.43	8.65	29.14	14.97	15.20	7.81

Table 3 Average of effective atomic number and electron density
(1023 electrons/gram)of coumarin dyes.

Compounds	1IPBC		4IP6MC	
Name of the process	$\langle Z_{\text{eff}} \rangle$	$\langle N_{\text{el}} \rangle$	$\langle Z_{\text{eff}} \rangle$	$\langle N_{\text{el}} \rangle$
Total non coherent	33.36	16.34	34.81	18.16
Total coherent	27.25	13.35	25.11	13.10
Pair electron	17.21	8.43	14.54	7.58
Pair nuclear	38.67	18.94	35.58	18.56
Photo electric	61.31	30.03	61.19	31.92
Incoherent	38.92	19.06	35.95	18.75
Coherent	60.20	29.49	59.79	31.19

Kerma relative to air

The variation of Kerma relative to air (K_a) of 1IPBC and 4IP6MC with photon energy 1 keV to 20 MeV is shown in Fig. 4. The K_a values were calculated using equation (10) and values of the selected organic molecules vary from 0.012 to 20 below 30 keV. K_a values attain maximum value around 100 at 40 keV, where photoelectric absorption is the dominating interaction process [38]. From 50 – 60 keV it starts decrease, attains constant value after 1 MeV [43]. It is clearly observed that Kerma depends on the chemical composition [44]. Later, kerma values decrease with increasing photon energy. The reason for such variation in kerma is the photoelectric cross section proportional to Z^4 –5 [45]. Above 200 keV photon energy, the compositional dependence of kerma is almost negligible. This is due to the dominance of the Compton scattering phenomenon [46], the interaction cross-section for which is essentially independent of atomic number Z .

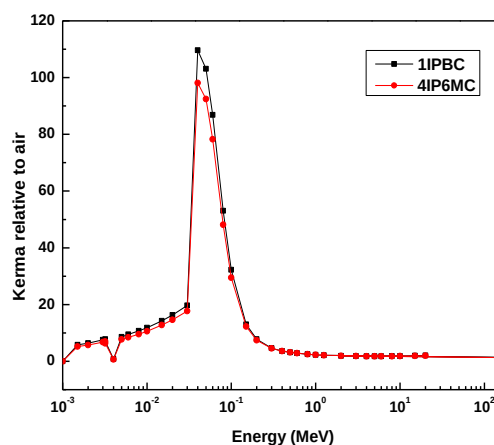


Fig. 4: Kerma relative to air for photon energy 1 keV-20 MeV of Coumarin dyes.

V. CONCLUSIONS

In this present work, the study has been undertaken to get information of the mass attenuation coefficients, effective atomic number Z_{eff} , electron density N_{el} and Kerma of 1IPBC and 4IP6MC using WinXCom. We can obtain the following conclusions from this study

- Mass attenuation coefficients, effective atomic number and corresponding electron density of 1IPBC and 4IP6MC have been calculated in the photon energy region 1 keV-100 GeV. There are three main photon-interaction processes photoelectric absorption, Compton scattering and pair production respectively.
- Effective atomic number and electron density of the selected coumarins were obtained for total and partial photon interaction processes i.e total photon interaction with coherent and without coherent, photoelectric absorption, coherent scattering, incoherent scattering, pair production in the electric and nuclear field.
- The maximum value of effective atomic numbers were observed in the low energy region $E > 0.5$ MeV where photoelectric absorption is the dominant process. At the K edges energies of the compounds more than a single values of Z_{eff} could be obtained due to non-uniform variation of mass attenuation coefficients.
- The minimum value of effective atomic numbers were observed in the intermediate energy region $2 < E < 400$ MeV, where Compton scattering is the main interaction process.

- Pair production is the predominant activity in the high energy zone, where the effective atomic number values have intermediate energies of less than 400 MeV. The N_{el} shares the same qualitative energy dependence as the Z_{eff} and is closely connected to it.
- Variation of 1IPBC and 4IP6MC's Kerma with photon energy ranging from 1 keV to 20 MeV where the predominant interaction process is photoelectric absorption.

VI. CONFLICT OF INTEREST

The author of this paper has no personal relationship with other organisation that could inappropriately influence the content of this paper.

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