ORIGINAL ARTICLE

Atomic Parameters of Some Commonly Used Liquid Crystals

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ABSTRACT

In the present work, different methodologies have been used to find the gamma energy dependence of two atomic parameters of three commonly used liquid crystals, 4-Cyano-4'-pentylbiphenyl (5CB), 4-heptyl-4'-cyanobiphenyl (7CB) and 4-n-nonyl-4'-cyanobiphenyl (9CB).The atomic parameters calculated as a function of gamma energy were the effective atomic number (Z_{eff}) and effective electron density (N_{eff}). This work helps to identify the crystal which is most sensitive to gamma energies compared to the other crystals, and compares the different methods used to calculate the atomic parameters. Three different methods have been used to find the dependence of effective atomic number of the crystals on gamma energy, namely: Direct, Direct-Z_{eff} and Auto- Z_{eff} Methods. But only two of the methods, Direct and Direct-$Z_{eff,}$ were used in this work to find the gamma energy dependence of effective electron density of the selected crystals because the Auto Z_{eff} method is not designed for calculating N_{eff}. The results of Direct and Direct-Z_{eff} methods are in good agreement with each other. The Z_{eff} as evaluated by Auto-Z_{eff} was lower than the Direct and Direct-Z_{eff} predictions in the higher gamma energy region (>10MeV). In the gamma energy region, approximately between 100keV and 10MeV, all the three methods predict that the Z_{eff} of the crystals are independent of the gamma energy. Finally, Z_{eff} decreases as we go from 5CB through 7CB to 9CB crystals. This means that liquid crystal 5CB is more affected by the radiation compared to 9CB. Therefore, the device furnished with 5CB crystal will have shorter life time inside reactor centers, accelerators or at any gamma radiation areas.

Keywords: Attenuation coefficients, Effective atomic number Z_{eff}, Effective electron density N_{eff}, 5CB, 7CB, 9CB liquid crystals

INTRODUCTION

Liquid crystals (LCs) are a state of matter having characteristics which lies between liquids and solids. The molecules of a liquid crystal have orientations like crystals in solids but can flow like liquid crystals. There are different phases of liquid crystals that can be differentiated from one another by their optical

properties. The study of liquid crystals began in 1888 when an Austrian botanist Friedrich Reinitzer observed that cholesteryl benzoate had two distinct melting points at 145.5 and 178.5 in degree Celsius. At the former, the crystal melts in to cloudy liquid and at the later it becomes clear liquid. Reinitzer is often credited with discovering liquid crystal phase. It is a thermodynamic stable phase characterized by anisotropy of properties without the existence of a three-dimensional crystal lattice. These are called mesophase as they lie in the temperature range between the solid and isotropic liquid phase. Liquid crystals are unique in their properties and uses.

As research into this field continues and their new applications are developed, liquid crystals play an important role in modern technology. In the last decade, their unique optical, electrical, electro-optic, and thermal properties have been exploited to a significant way. Digital watches and calculators equipped with liquid crystal displays (LCD's) have recently made their debut in the electronic market. The large-scale use of LCD's in a variety of other applications requiring reliable, low-power digital displays is imminent.

Liquid crystals are going to become the first electro-optic materials to find widespread application for commercial use (Collings & Hird, 1997; Castelleno, 2005; Jan et al., 2012; Pankaj, 2013; Quiny, 2017; Petrov et al., 2017). Due to low power requirement, such devises find wide applications in space craft's going to the outer space. Also because of their ruggedness, they find applications in control panels of nuclear installations like atomic reactors, and accelerators.

Liquid crystals are also extensively used in various instruments as displays where they are exposed to relatively high dose of nuclear radiations like gamma rays. The absorption of gamma rays in such materials depends upon effective atomic number (Z_{eff}) and effective electron density (N_{eff}) of the material. If a liquid crystal changes its atomic property due to the absorption of gamma rays, radiation devises furnished with such liquid crystal will have short life time. Therefore, the two parameters (Z_{eff} and N_{eff}) are most important in the study of destructive effect of gamma rays of different energies on liquid crystals. In the present work, the atomic properties Z_{eff} and N_{eff} of three most commonly used liquid crystals as a function of gamma energy were evaluated to see the consistency of the results with different methods and select the crystal most sensitive to the gamma energy.

The first liquid crystal was 4-Cyano-4'-pentylbiphenyl with the chemical formula $C_{18}H_{19}N$ and it is commonly named as 5CB (Ramesh et al., 2013; Shin-Pou et al., 2016). The second was 4-heptyl-4'-cyanobiphenyl with chemical formula $C_{20}H_{23}N$ and common name 7CB (Marinov et al., 2015; Hadjichistov et al., 2017). The third liquid crystal considered was 4-n-nony l-4'-cyanobiphenyl with chemical formula $C_{22}H_{27}N$ and common name 9CB (Roy & Mukhopadhyay, 2016). All the three liquid crystals find wide applications in the various electronic panels.

To the best of our knowledge, no such calculations are available in literature for any of these liquid crystals.

MATERIAL AND METHODS

The Z_{eff} and N_{eff} of the three crystals (5CB, 7B and 9CB) as a function of gamma energy were calculated using the following methods.

Direct Method

This method uses the concept of gamma attenuation when it passes through a

material media (Madhusudhan Rao et al., 2016). Intensity (I) of the attenuated beam is related to its unattenuated beam intensity (I_0) by the Lambert – Beers law given in Eq. 1.

$$I = I_0 e^{-\mu x} \quad (1)$$

Where x is the thickness of the material in 'cm' and μ is its linear attenuation coefficient in cm^{-1}. The mass attenuation coefficient of the material (μ_m) was obtained from the value of its linear attenuation coefficient and density (ρ) of the material as given in Eq.2 (Madhusudhan Rao et al., 2016).

$$\mu_m = \frac{\mu}{\rho} \quad (2)$$

Since the materials under study (5CB, 7B and 9CB) are composite materials, total μ_m is given by the relation in Eq. 3 (Madhusudhan Rao et al., 2016). Where w_i is the weight fraction if the i^{th} element.

$$\mu_m = \sum_i w_i \frac{\mu_i}{\rho_i} \quad (3)$$

To find the total weight fraction of each of the crystals under study, an equation of weight fraction for composite materials, Eq.4 was used.

$$w_i = \frac{n_i A_i}{\sum_i n_i A_i}$$

Satisfying $\sum w_i = 1$ (4)

Where A_i and n_i are the atomic weight and the number formula units of the i^{th} element in the crystal compound, respectively.

The WinXCom software was used to obtain mass attenuation coefficient of the liquid crystals understudy (Gerward *et al*., 2004).

The results obtained from calculations of mass attenuation coefficients were used to find for the total atomic cross-section σ_t using Eq. 5 (Singh and Gerward, 2002).

$$\sigma_t = \frac{\mu_m M}{N_A} \quad (5)$$

Where M is the atomic mass of the material and N_A is Avogadro's number.

For each of the liquid crystals the total electronic cross sections which depend on the total mass attenuation coefficient were obtained using Eq. 6. Total electronic cross-section σ_e for a particular liquid crystal and its total atomic cross sections are related as shown in Eq. 6 (Manohara et al., 2008).

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} (\mu_m) = \frac{\sigma_t}{Z_{eff}} \quad (6)$$

Where f_i is the fractional abundance of the element i with respect to the number of atoms such that $\sum_i f_i = 1$

Finally, the ratio of total atomic cross-section σ_t and total electronic cross-section σ_e, as in Eq. 7, was used to find the effective atomic number of the crystals.

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

Number of electrons per unit mass (effective electron density) was determined using the relation given in Eq. 8 (Gowda, 2005; Manohara *et al*., 2008).

$$N_{eff} = \frac{\mu_m}{\sigma_e} \qquad (8)$$

Direct-Z_{eff} Method

The software Direct-Z_{eff} was developed by Adam and Tanfer (2014) for the purpose of finding Z_{eff}, Neff and μ_m in the energy range of 1 keV to 1GeV. In the present investigation, this software was used to calculate Z_{eff} and N_{eff} as a function of incident gamma rays energy for the three crystals and compare the results with the Direct Method. The input parameters for this software were the elements symbol in the compound, atomic number (Z) of the element and their fractional composition.

Auto-Z_{eff} Software

In this software, Z_{eff} is determined by considering the co-relation between atomic cross-section and atomic number (Taylor et al., 2012). The software constructs a matrix of cross-sections for atomic numbers (Z) between 1 to 100 and gamma energy (E) between 10 to 10^6 keV. The cross-sections for the crystals under study (poly-elemental materials) were calculated via linear additivity by the software. These cross-section values were then compared with the cross-section matrix as a function of Z per each gamma energy. Effective atomic numbers were extracted by interpolation of Z values between adjacent cross-sectional data. Similar to the parameters during the Direct-Z_{eff} software, the inputs in this software are the elements symbol in the compound, atomic number (Z) of the element and their fractional composition (weight fraction).

The drawback of this software is that it does not evaluate effective electron density N_{eff}.

RESULT AND DISCUSSION

The Z_{eff} Calculation

Variation of Zeff as calculated by Direct method, Direct-Z_{eff} software and Auto-Z_{eff} software for crystals 5CB, 7CB and 9CB are shown in the graphs displayed below (Fig. 1).

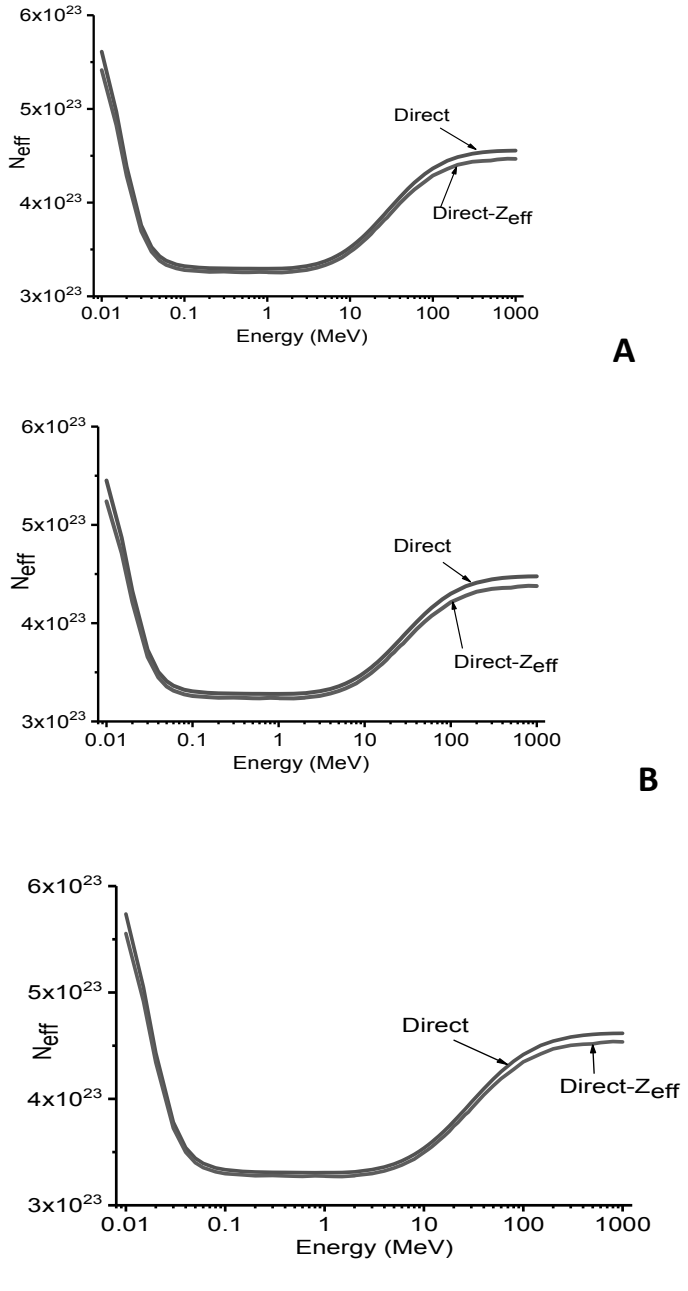


Figure 1. N_{eff} as a function of energy for 5CB (A), 7CB (B), and 9CB (C) liquid crystal.

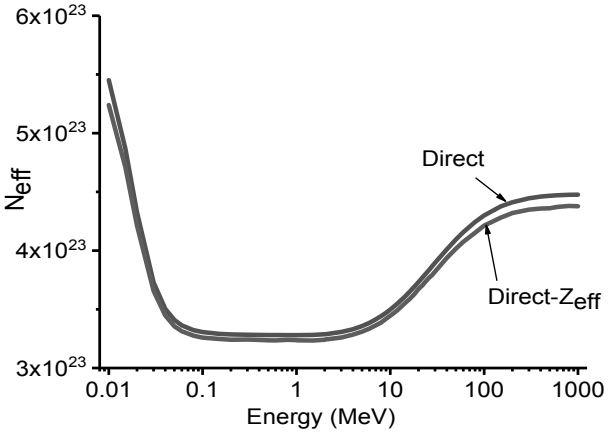
From the graphs shown in the Figs. 1 to 3, at low energies < 0.01 MeV, Z_{eff} reaches its local maximum in the energy range below 1GeV and it rapidly decreases in the energy range between 0.01 and 0.1MeV. This is an evident that the effect of the gamma energy on the Z_{eff} of the crystals begins from the value as low as 0.01MeV. Furthermore, in the energy range between 0.1 to about 10 MeV, Z_{eff} remains almost constant. In this region, Z_{eff} is independent of the gamma energy as predicted by other methods, the Power Law and software XMuDat method. These two methods describe that Z_{eff} is independent of energy of incident gamma rays in all energy region of the gamma (Murty, 1965; Nowotny, 1998). Beyond this energy, it increases relatively slowly and then it levels off.

As can be seen from the figures, Z_{eff} calculated by Direct and Direct-Z_{eff} methods agree well up to highest energy. Calculations of Auto-Z_{eff} agree with the other two calculations only up to 20 MeV. For energies > 20 MeV, the predictions of Auto-Z_{eff} are lower than the other two methods. At higher energy this deviation is as large as about 14%. The reason for such a large deviation of the predictions of Auto-Z_{eff} is not clear. In their paper, Taylor et al. (2012) tested this software up to gamma energy of 5 MeV comparing with experimental data. Their findings showed that the Auto-Zeff software calculations were agreed quite well with experimental values for energies up to 5 MeV.

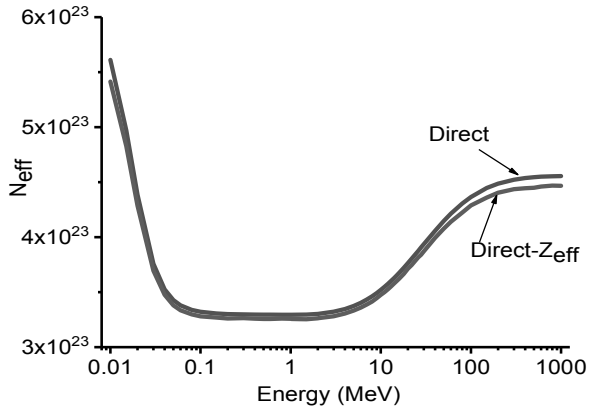
In the present work, experimental data on Z_{eff} and N_{eff} of the liquid crystals as a function of gamma energy were not obtained (or not available), thus calculations have been cross checked with three different methods and the data obtained by Auto-Z_{eff} software at higher gamma energies were not been considered.

N_{EFF} CALCULATION

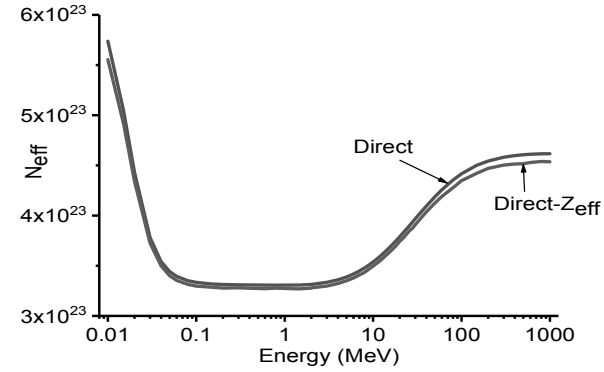
Effective electron density as calculated using Direct method and Direct-Z_{eff} software for 5CB, 7CB and 9CB crystals are shown below (Fig. 2).



A



B



C

Figures 2 N_{eff} as a function of energy for 5CB (A), 7CB (B), and 9CB liquid crystals

Calculation for N_{eff} using Auto-Z_{eff} software has not been made since the software is not designed for such calculation. Similar to the dependence of Z_{eff} on the gamma energy discussed earlier, N_{eff} attains its maximum value at low energies below 0.01MeV and the variation of N_{eff} as a function of incident γ-energy divided in to four regions. In the first region, with energy range of 0.01 to 0.1 MeV ($0.01 < E < 0.1$ MeV), N_{eff} decreases faster indicating that the effect of gamma energy at low energies is to reduce N_{eff} of the liquid crystals. In the second region, 0.1 to about 10 MeV, N_{eff} becomes nearly constant. In the third region, approximately in $10 < E < 100$ MeV, it increases slowly and in the final region $E > 100$ MeV, its value becomes almost constant.

Both calculations made for Z_{eff} and N_{eff} in the current study depend on the cross section of the three mechanisms of interaction of gamma with the electrons of the crystals. Gamma interaction in the low ($0.01 < E < 0.5$ MeV), intermediate ($0.5 <$

E < 5 MeV) and high energy (E > 5 MeV) regions are dominated by the interactions of photo electric effect, Compton scattering, and pair production, respectively.

In order to explain this behavior of Z_{eff} and N_{eff} as a function of γ-ray energy, we have to see the relative importance of the partial γ-ray interaction processes with matter. In low energy region, cross section for photo electric effect decreases as $\frac{1}{E^{3.5}}$. Compton-effect is negligibly small and pair production does not take place in this energy region. The values of Z_{eff} and N_{eff} also decrease almost in the same manner as photo electric cross section.

In the intermediate energy region, cross section for Compton scattering directly proportional to E and cross section for photo electric effect decreases as $\frac{1}{E}$. Cross section for pair production increases as $log_e(E)$. The net result is that total photon interaction cross section remains almost constant in the region. Therefore, the values of Z_{eff} and N_{eff} practically remain constant in the region. The constant values of Z_{eff} in this region are 3.58 for 5CB, 3.45 for 7CB and 3.35 for 9CB crystals in the present calculation.

Finally, in the high energy range cross sections for photo electric effect and Compton scattering are negligibly small while pair production cross section increases as $log_e(E)$. This increase is very slow and also it almost saturates for E > 100 MeV, Z_{eff} and N_{eff} also show similar behavior in this energy range. According to the present calculation at high energy region, Z_{eff} attains almost constant values of 4.86 for 5CB, 4.77 for 7CB and 4.68 for 9CB, respectively.

CONCLUSION

According to the present calculation, the predictions of values of Z_{eff} for all the three crystals, between energy values of 0.02 to 20 MeV, with the three methods (Direct, Direct-Z_{eff} and Auto-Z_{eff}) are in a good agreement with each other. However Z_{eff} calculated by Direct method is well reproduced by Direct-Z_{eff} software for almost at all the energies. The Z_{eff} as evaluated by Auto-Z_{eff} for energies above about 20 MeV deviates highly from the other two methods.

The effective electron density predictions of both Direct and Direct-Z_{eff} methods agree very well. However, at higher energies (E > ~ 200 MeV) the values start deviating from one another though the deviations are small (between 2 to 4%).

Finally, Z_{eff} decreases as we go from 5CB through 7CB to 9CB. As the interaction of γ-photons due to photoelectric effect, Compton scattering and pair production increases with increasing Z, so 5CB is more prone to radiation damage compared to 9CB. This means that liquid crystal displays using 9CB may survive higher radiation environment.

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