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Density Functional Theory (DFT) Study of a Binary Mixture of MBBA and PAA Liquid Crystal for THz Application

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Abstract

The present scenario expresses the electro-optical effect of abinary mixture of MBBA and PAA liquid crystal studied under the impact of the electric field in THz frequency. The binary mixture has a negative order parameter, negative birefringence, and a nematic phase stability under such an electric field. The refractive index remains constant at high THz frequency. The director angle is sensitive to THz frequency, contributing to the maximum fluctuation. The atomic contribution of a binary mixture is approximately equal to the molecular contribution. The binary mixture has a remarkably high bandgap. The C-H, O-C, C-N atom stretching, and wagging of alkyl chain contribute to the dipolar strength of the binary mixture.

Keywords:bandgap, binary mixture MBBA-PAA, DFT, electric field (THz), electro-optical effect

Introduction

The MBBA (*N-(4-Methoxybenzylidene)-4-butylaniline*) liquid crystal (LC) was first synthesized by Hans Kelker in 1969 and expressed the nematic phase at room temperature. In the year 1970s, the MBBA LC was used for the first time by the United Kingdom for the liquid crystal display (LCD). The moisture enters the LCD and damages the alignment of LC under the influence of the electric field due to the hydrolysis problem. Therefore MBBA LC no longer expresses the alignment of molecules and also exhibits a negative dielectric anisotropy defined as $\Delta\varepsilon = \varepsilon_{\text{II}} - \varepsilon_{\perp}$. The amino linkage group (≡N) is responsible for the negative dielectric anisotropy. In 1973, Dr. George Gray from the University of Hull synthesized *4-Cyano-4'-pentylbiphenyl* (5CB) LC the first time; 5CB LC was also commercialized by the UK industry. The 5CB LC was moisture free and also hada positive dielectric anisotropy. The 5CB was highly polar and perfectly maintained the alignment of molecules; however, MBBA demonstrates poor alignment of all the molecules. Therefore, 5CB was the superior alternative of MBBA LC. The MBBA LC was aligned along the surface under the impact of the electric field. The nematic phase is sensitive to the surface due to substantial induced disorder. The PAA (*para-azoxyanisole*) is a rod-like nematic LC, which also has a negative dielectric anisotropy [1]. Shibaev *et al*. [2] reported that the MBBA is a rod-like nematic phase LC, that is remarkably sensitive to the environment; therefore, MBBA can be used in environmental gas sensor applications. Lee at al. [3] investigated LED panels and found that PAA LC is remarkably sensitive to the tactile force magnitudes (express ripple propagation on screens); however, MBBA is insensitive to the tactile force magnitudes. Bouligand *et al*. [4-5] studied a mixture of MBBA and PAA which expresses the stable nematic phase. Diezat al. [6] revealed that the binary mixture of MBBA and PAA exhibits the broad range nematic phase with perfect alignment of molecules.

The PAA is less viscous compared with MBBA. The MBBA is sensitive to the low-frequency dependence characteristics and controlled by the molecular diffusion mechanism due to the proton spin-lattice relaxation in the nematic phase. However, the PAA exhibits high frequency dependence characteristics through the order fluctuation mechanism; thus, the binary mixture is chosen for the current work. The MBBA and PAA LC are predominant; the molecular interaction through

wagging of the alkyl chain and alkyl chain is temperature dependent (chain length increased with the reduction in temperature) [7]. The nematic phase of PAA LC maintains stability at substantially high Larmor frequency due to fluctuations of the director angle [8]. The order parameter of MBBA LC approached 0.6; but the binary mixture of MBBA and PAA reduced the order parameter to 0.54. The MBBA LC molecules are useful for the microwave heating effects, which are widely employed in the enzymatic reactions, acceleration of organic compounds, and polymerization [9]. The PAA LC behaves as a stimuli-responsive sensor, as mentioned by Sulayman [10]. PAA and MBBA are combined in the current study to function as sensing application devices. Takehisa *et al*. reported that the doping of MBBA LC material enhances its the porosity responsible for the sensing and filtering applications [11]. The PAA LC has stimuli-responsive transition as well as optical anisotropic properties [12]. Mihai *et al*. revealed that reported the MBBA enhances the birefringence of mixtures thus modifying the birefringence in the present work [13].

The electro-optical properties in the present work were calculated under the influence of terahertz (THz) frequency range with a binary mixture of MBBA and PAA LC. The MBBA and PAA LC are suitable for the low and high-frequency ranges, respectively; however, the binary mixture of PAA LC maintains the low to high THz frequency. The electric field in THz frequency was applied to the binary mixture and the optical properties, which are suitable for the different THz application devices were calculated.

Computational Methodology

The binary mixture of MBBA and PAA LC molecules are optimized by the NWChem Software [14] using density functional theory (DFT) method B3LYP [15-16] and M062X [17] with 6−31G** basis set [18]. After the simulation of binary mixture, the electric field (a.u) is applied to the binary mixture along the molecular axis (x-axis) and perpendicular (y-axis). The range of the applied electric field is 0.0000 atomic unit (a.u.) to 0.1500 a.u with an interval of 0.0020 a.u, where 1 a.u.=5.14 × 10^9 V/m or 1 a.u.= 6.57968 × 10^{15} Hz [19]. The molecular polarizability of a binary mixture is calculated after the application of an electric field. Along the x-axis, molecular polarizability of the binary mixture is considered as extraordinary molecular polarizability (α_e), and along the y-axis is considered as ordinary molecular polarizability (α_o). With the help of α_e and α_o, the refractive index, birefringence, director angle, and order parameter of the binary mixture are calculated on the basis of the formula provided below [20-21. where β, α, and μ equivalent to the components of the first-order hyperpolarizability (b), polarizability (a) and dipole moment (c), average polarizability (d, e, f) respectively,

$$\alpha = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad \text{(a)}$$

$$\beta = \left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})^2\right]^{1/2} \quad \text{(b)}$$

$$\mu = (\mu_x{}^2 + \mu_y{}^2 + \mu_z{}^2)^{1/2} \quad \text{(c)}$$

$$\Delta\alpha = 2^{-1/2}\left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2\right]^{1/2} \quad \text{(d)}$$

$$\Delta\tilde{\alpha} = \alpha_e - \alpha_o \quad \text{(e)}$$

$$\Delta\tilde{\alpha} = S\Delta\alpha \quad \text{(f)}$$

Order Parameter (S) [1]:-

$$S = \frac{\alpha_e - \alpha_o}{\alpha_e + \alpha_o}, \quad (1)$$

Birefringence (Δn) [20]:-

$$\Delta n = \frac{(\alpha_e - \alpha_o)}{6.3631}\left[R^3 - \left(\frac{2\alpha_o + \alpha_e}{20.244}\right)\right]^{-1}, \quad (2)$$

where, R is the radius of the binary mixture.

Magic angle (θ) [1]:-

$$\theta = \cos^{-1}\left[\frac{(2S+1)}{3}\right] \quad (3)$$

Refractive index (n) [1,20]:-

$$\alpha = \frac{2\alpha_o + \alpha_e}{3}, (3.1) \qquad \gamma_e = \alpha + \frac{2(\alpha_e - \alpha_o)}{3S}, (3.2) \qquad \gamma_o = \alpha - \frac{(\alpha_e - \alpha_o)}{3S}, (3.3)$$

$$n_e = \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1-\frac{4\pi N\alpha}{3}} + \frac{(4\sqrt{10}/15)\pi NS(\gamma_e - \gamma_o)}{1-\frac{4\pi N\alpha}{3}}, (3.4)$$

$$n_o = \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1-\frac{4\pi N\alpha}{3}} - \frac{(2\sqrt{10}/15)\pi NS(\gamma_e - \gamma_o)}{1-\frac{4\pi N\alpha}{3}}, (3.5)$$

$$n = \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1-\frac{4\pi N\alpha}{3}}, \quad (4)$$

where N=300 is the number of binary mixture.

Results and Discussion

The DFT method B3LYP is predominant in the atomic contribution of the binary mixture; however, the M062X method is predominant in the molecular contribution of the binary mixture. The present work indicates the atomic and molecular contributions of the binary mixture. Under the impact of THz frequency, the molecular contribution of the binary mixture is predominant for all the optical characteristics. The optimized geometry of MBBA and PAA LC is shown in Figure 1.

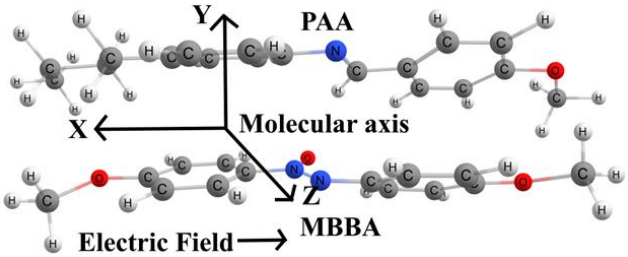

Figure 1. Optimized Geometry of MBBA and PAA LC by DFT Methodology

Order parameter. The order parameter is calculated by DFT methodology using Equation 1, as shown in Figure 2. Kobinata *et al*. [22] reported that the order parameter of MBBA is 0.60. However, in the present work, the order parameter decreases to 0.54 because of the order fluctuation of PAA LC. The DFT methods B3LYP and M062X expressed the same nature of characteristics; therefore, atomic contribution can be predicted similarly to the molecular contribution with the different values. Both methodologies predicted nematic phase stability under the impact of the electric field in THz frequency. Chandrasekhar *et al*. [23] found that the experimental and theoretical order parameter of PAA LC are 0.55 and 0.43 respectively. Therefore experimental and theoretical pieces of evidence are predicted to support the molecular and atomic contributions, respectively. The binary mixture also expresses the re-entrant nematic phase at a high frequency. Through the M062X method, the maximum

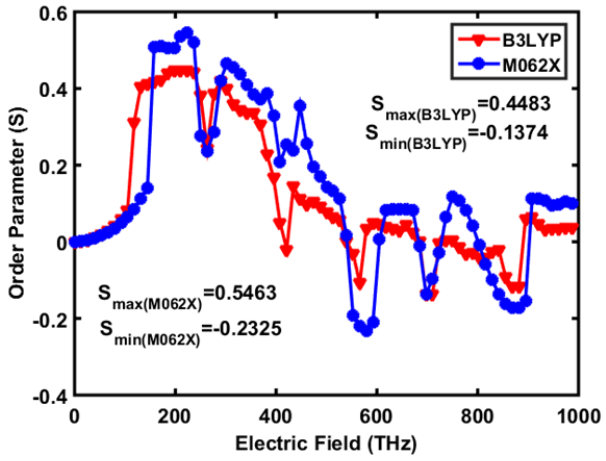

Figure 2. Order Parameter Calculated by DFT Methodology under the Impact of the Electric Field in THz Frequency

and minimum order parameters are 0.54, and −0.23, respectively; through the B3LYP method, the maximum and minimum order parameter are 0.44, and −0.13, respectively. The order parameter characteristics areused to express the nematic to the isotropic phase transition. The binary mixture is sensitive to the electric field which leads to the continuous fluctuation of the order parameter. Above 0.14 a.u. electric field, the binary mixture is finally converted to the isotropic phase.

Birefringence. The birefringence is calculated by DFT methodology using Equation 2, as shown in Figure 3. Shibaev *et al*. [2] reported that the birefringence of MBBA LC is 0.30; however, the birefringence reductionof a binary mixture in the present work 0.25 due to the conversion of this mixture to the dense property. The optical property birefringence is predominant in the molecular contribution. Thenematic phase stability is also observed in the birefringence characteristics. Pan *et al*. [24] reported that the birefringence of 5CB LC in THz frequency is equal to 0.20; however, the birefringence of a binary mixture is 0.25, in the present work. The binary mixture maintained low birefringence at a high THz frequency range. The re-entrant behavior of molecules is also observed in the birefringence characteristics. Through the DFT method M062X, the maximum and minimum birefringence are 0.25, and −0.11, respectively. Meanwhile, the B3LYP method expresses maximum and minimum birefringence are 0.17, and −0.07, respectively. Leenhouts *et al*. [25] reported the existence of MBBA LC birefringence between 0.20 and 0.22, while the birefringence enhanced due to director fluctuation of PAA LC in the present work.

Director angle. The director angle is calculated by DFT methodology using Equation 3, as shown in Figure 4. The director angle fluctuated under the impact of the THz frequency range. The DFT method M062X yielded maximum and minimum direct or angle of 65° and 33°, respectively; meanwhile, by the B3LYP method produced maximum and minimum director angle of 60° and 37°, respectively. The M062X method expresses more significant fluctuation compared with B3LYP. Therefore, molecular contribution is more predominant compared with an atomic contribution. The director angle also indicates the nematic phase stability. The director angle fluctuation represents it is susceptible to the THz frequency thus, this fluctuation is also applicable for the sensing applications.

Refractive index. The refractive index is calculated by DFT methodology using Equation 4, as shown in Figure 5. The THz spectroscopy is a powerful tool for describing the phase transition and dichroism of liquid crystals. Nishizawa *et al*. [26] found that the MBBA LC expresses strong dichroism in the THz frequency, which corresponds to the IR absorption caused by C–H atom stretching. Roger Chang [27] revealed that the average refractive

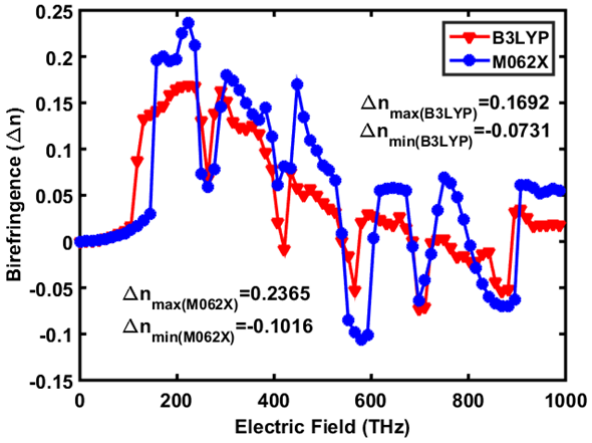

Figure 3. Birefringence Calculated by DFT Methodology under the Impact of the Electric Field in THz Frequency

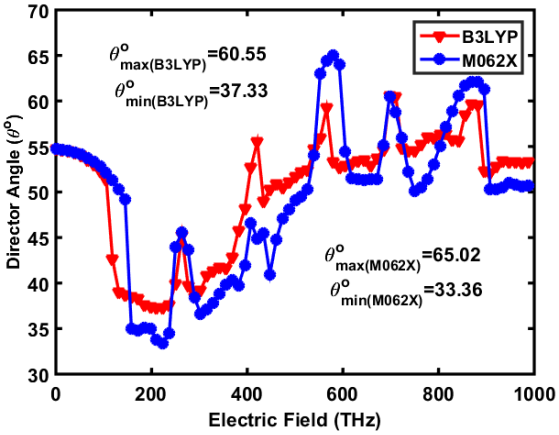

Figure 4. Director Angle Calculated by DFT Methodology under the Impact of the Electric Field in THz Frequency

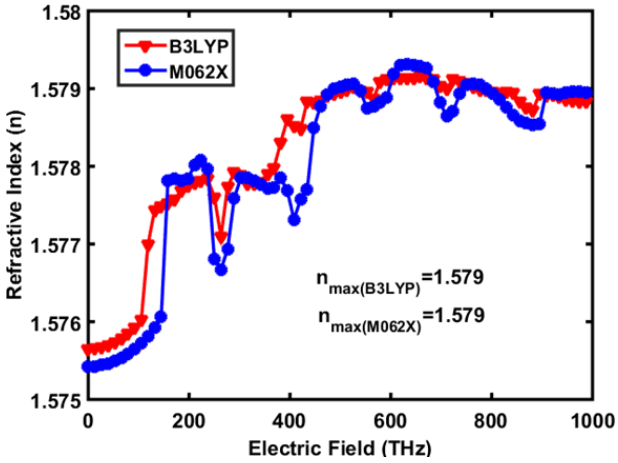

Figure 5. Refractive Index Calculated by DFT Methodology under the Impact of the Electric Field in THz Frequency

index of MBBA LC exists between 1.76 to 1.54, while the average refractive index of a binary mixture is 1.57 in the present work. For the refractive index characteristics, the atomic and molecular contributions were found to be equal but with different values. The nematic phase stability was observed at low THz frequency range in the refractive index characteristics. The refractive index remains constant at the higher frequency, which is suitable for the THz applications. Kumar *et al*. [28] indicated that the DFT (B3LYP) methodology is most ideal for organic compounds. The current work also reveals that organic compounds (liquid crystal) are used for the theoretical prediction.

Bandgap and dipolar strength. The highest occupied molecular orbital-lowest unoccupied molecular orbital bandgap of a binary mixture is 5.19 eV, as shown in Figure 6. The dipole moment of a binary mixture is 7.61 Debye. The binary mixture has suitable dipolar strength, as shown in Figure 7. The C-H, O-C, C-N atom stretching, and wagging of alkyl chain contribute to the dipolar strength of the binary mixture as shown in Figure 7. Vilfan *et al*. [7] reported that the wagging of alkyl chain mostly contributes to the intermolecular interaction of a binary mixture rather than the translation motion of the molecules; the present work theoretical prediction also supports the experimental evidence. The molecular spectroscopy of binary mixture MBBA and PAA is given in Table 1. The table indicates that scissoring of hydrogen atom of MBBA and PAA contributed maximum dipolar strength at the frequency of 1236 THz.

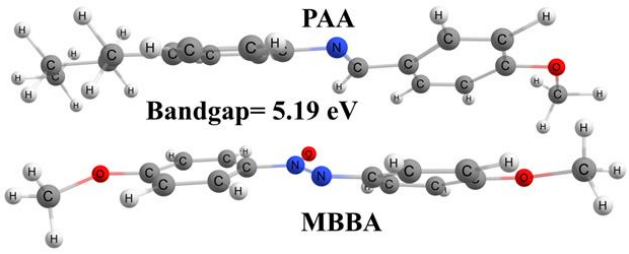

Figure 6. Molecular Bandgap Calculated by DFT Methodology (M062X) of Binary Mixture MBBA-PAA LC

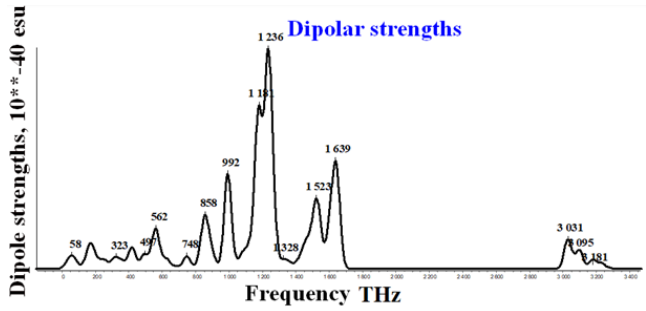

Figure 7. Dipolar Strength of Binary Mixture Calculated by DFT Methodology (M062X)

Table1. Molecular Spectroscopy of Binary Mixture MBBA and PAA

Frequency (THz)	Mode of Vibrations
562	O-C Scissoring (in plane bending) in PAA
858	H twisting (out of plane bending) in PAA
992	O-C stretching in PAA
1181	H scissoring in MBBA
1236	H scissoring in MBBA or PAA
1639	C-C stretching in PAA
1523	In plane rocking in PAA
3031	Asymmetric stretching in PAA and MBBA

Conclusion

In the present scenario, the binary mixture expresses an electro-optical effect under the impact of the electric field in THz frequency. The nematic phase is stable under THz frequency and expresses re-entrant nematic phase transition. The binary mixture reveals positive and negative order parameters and birefringence. The binary mixture behaves as an insulator due to a large bandgap. The C-H, O-C, C-N atom stretching, and wagging of alkyl chain contribute to the dipolar strength of the binary mixture. The director angle sensitive to the THz frequency thereby inducing maximum fluctuation. The scissoring of hydrogen atoms of MBBA and PAA liquid crystal contributed maximum dipolar strength at the frequency of 1236 THz. The refractive index remains constant in THz frequency therefore, this index is suitable for different applications in the THz frequency.

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