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DFT-Based Study of Physical, Chemical and Electronic Behavior of Liquid Crystals of Azoxybenzene Group: \( p\)-azoxyanisole, \( p\)-azoxyphenetole, ethyl-\( p\)-azoxybenzoate, ethyl-\( p\)-azoxyccinnamate and \( n\)-octyl-\( p\)-azoxyccinnamate

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Abstract: The present work describes the geometry and electronic structures of liquid crystals of azoxybenzene group and their reactivity with respect to molecular properties: total energy, ionization potential, electron affinity, HOMO energy, LUMO energy, electronegativity, hardness and dipole moment. Literature shows that mesomorphism depends particularly on the nature of terminal groups and their linkages with parent molecule. And thus, substitution of terminal groups can help to fine tune the liquid crystal behavior and also their applications. In this work the effect of four terminal groups of same and diverse nature has been studied. For the study, the molecular modeling and geometry optimization of the compounds have been performed on workspace program of CAChe Pro 5.04 software of Fujitsu using DFT method.

Keywords: Nematic liquid crystal, Azoxybenzene, DFT, Molecular properties

1. Introduction

All highly deformable materials (soft matter) including polymers, collides and surfactant solutions are studied in liquid-crystal physics and have novel technological applications [1, 2]. Liquid crystalline behaviors of materials depend on chemical structure and physical properties of structural unit [3]. At present theoretical conclusions are available, based on extensive experimental data regarding mesomorphism of low molecular weight mesophases, depending on the structure of molecules, particularly on the nature of terminal groups and linkages [4]. This enables to synthesize new compounds with desired liquid crystalline properties. \( p\)-Azoxyanisole (PAA) is an organic compound. In a solid state, it appears as a white powder, but when heated it forms a liquid crystal. As one of the first known and most readily prepared liquid crystals, PAA has been played an important role in the development of liquid crystal displays [5, 6]. Presently, a number of azoxy based liquid crystals are well known. Some of azoxybenzene-based liquid crystals, listed in Table-1, belonging to nematic class are \( p\)-azoxyanisole, \( p\)-azoxyphenetole, ethyl-\( p\)-azoxybenzoate, ethyl-\( p\)-azoxyccinnamate and \( n\)-octyl-\( p\)-azoxyccinnamate. In our previous work, we have described some behavior of these liquid crystals based on (i) partial atomic charges [7], (ii) frontier orbital densities [8] and (iii) bond properties viz., bond length, bond order and bond angle [9]. In this work, we present geometry and electronic structure of above liquid crystals based on molecular properties: total energy, ionization potential, electron affinity, HOMO energy, LUMO energy, electronegativity, hardness and dipole moment.

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2. Materials and Methods

The study materials of this work are listed in Table 1. For present study the three dimensional modeling and geometry optimization of all the compounds have been done in DGauss using the DFT B88-PW91 GGA functional with the DZVP basis sets [10, 11]. The application of DFT has given a new concept to chemical system [12]. The DFT based calculations of above parameters were performed with CAChe software and results are tabulated in Table 2 to Table 10.

Table 1. List of azoxy-based liquid crystal (LC)

| No. | X          | Compd. Name          |
|-----|------------|----------------------|
| 1   | –OCH₃      | p-azoxyanisole       |
| 2   | –OC₂H₅     | p-azoxyphenetole     |
| 3   | –COOC₂H₅   | ethyl-p-azoxybenzoate|
| 4   | –CH=CH-COOCC₂H₅ | ethyl-p-azoxyccinnamate |
| 5   | –CH=CH-COOCC₈H₁₇ | n-octyl-p-azoxyccinnamate |

3. Results and Discussion

If p-azoxyanisole is treated as reference compound (RC) then the study shows that replacement of –OCH₃ group of RC by –OC₂H₅, –COOC₂H₅, –CH=CH–COOCC₂H₅ and –CH=CH–COOCC₈H₁₇ groups formed p-azoxyphenetole, ethyl-p-azoxybenzoate, ethyl-p-azoxyccinnamate and n-octyl-p-azoxyccinnamate, respectively. Molecular properties provide essential information of a molecule with respect to its physical, chemical and electronic performance. For sake of simplicity the study of above liquid crystals with respect each molecular property is described in different heads as given below.

3.1. Total Energy

The structure and stability of a molecule is determined by the total energy \( E \) of the molecule [13]. Total energy can be partitioned as follows.

\[
E = T_n + T_e + V_{nn} + V_{ne} + V_{ee}
\]

where \( T_n \) is the kinetic energy of all nuclei, \( T_e \) is the kinetic energy of all electrons, \( V_{nn} \) the potential energy of all Coulomb interactions between the nuclei, \( V_{ne} \) the potential energy of Coulomb interactions between the nuclei and the electrons, and \( V_{ee} \) the potential energy of all Coulomb interactions between the electrons. The total energies of the above LCs were evaluated and are reported in Table 2. A reference to the table indicates that the total energy of RC is \(-877.067\) hartree. On replacement of –OCH₃ group of RC by –OC₂H₅, there is an increase of \(78.635\) hartree energy of the resulted compound, \( p \)-azoxyphenetole. Similarly, replacement of –OCH₃ group of RC by –COOC₂H₅, –CH=CH–COOCC₂H₅ and –CH=CH–COOCC₈H₁₇ groups increases the E of the resulting compounds. This is also demonstrated by Figure 1.

3.2. Frontier Orbital Energies

Energies of the highest occupied molecular orbital (\( \varepsilon \text{HOMO} \)) and lowest unoccupied molecular orbital (\( \varepsilon \text{LUMO} \)) are very popular quantum chemical descriptors. It has been
shown that these orbitals play a major role in governing many chemical reactions and determining electronic band gaps in solids; they are also responsible for the formation of many charge transfer complexes [14]. According to the frontier molecular orbital theory (FMO) of chemical reactivity, the formation of a transition state is due to an interaction between the frontier orbitals (HOMO and LUMO) of reacting species. Thus, the treatment of the frontier molecular orbitals separately from the other orbitals is based on the general principles governing the nature of chemical reactions. The HOMO energies of the above LCs were evaluated and are reported in Table 3. A reference to this table indicates that the HOMO energy of RC is -4.994. On replacement of –OCH₃ group of RC by –OC₂H₅, there is an increase of 0.053 eV value of HOMO energy of the resulted compound, p-azoxyphenetole. Similarly, replacement of –OCH₃ group by –COOC₂H₅ (compd. no. 3) shows a decrease (0.969 eV) in the value of HOMO energy. Thus, ethyl-p-azoxybenzoate has lower value of HOMO energy of 1.022 eV than the former compounds. On further replacement of –OCH₃ group by –CH=CH–COOC₂H₅ (ethyl-p-azoxycinnamate) shows a decrease in the value of HOMO energy with respect to compd. no. 1 and 2 but an increment in respect to 3. Finally, replacement of –OCH₃ group by CH=CH–COOC₂H₃: (n-octyl-p-azoxycinnamate) shows an abnormal decrease in the HOMO energy. The decreasing order of HOMO energy of above LCs for electrophilic attack is p-azoxyphenetole > p-azoxyanisole > ethyl-p-azoxycinnamate > ethyl-p-azoxybenzoate > n-octyl-p-azoxycinnamate (Figure 2).

Table 2. Total energy of azoxy-based LC

| No. | Compd. Name          | E (Hartree) |
|-----|----------------------|-------------|
| 1   | p-azoxyanisole       | -877.067    |
| 2   | p-azoxyphenetole     | -955.702    |
| 3   | ethyl-p-azoxybenzoate| -1182.402   |
| 4   | ethyl-p-azoxycinnamate| -1337.230  |
| 5   | n-octyl-p-azoxycinnamate| -1387.760 |

Figure 1. Graph showing effect of substitution on total energy of the compound

Table 3. Energy of highest occupied molecular orbital of azoxy-based LC

| No. | Compd. Name          | εHOMO (eV) |
|-----|----------------------|------------|
| 1   | p-azoxyanisole       | -4.994     |
| 2   | p-azoxyphenetole     | -4.941     |
| 3   | ethyl-p-azoxybenzoate| -5.963     |
| 4   | ethyl-p-azoxycinnamate| -5.745    |
| 5   | n-octyl-p-azoxycinnamate| -75.532  |
The LUMO energies of the above LCs were evaluated and are also reported in Table 4. A reference to this table indicates that the LUMO energy of RC is -2.718 eV. On replacement of \(-\text{OCH}_3\) group of RC by \(-\text{OC}_2\text{H}_5\), there is an increase of 0.05 eV value of LUMO energy of the resulted compound, \(p\)-azoxyphenetole. Similarly, replacement of \(-\text{OCH}_3\) group by \(-\text{COOC}_2\text{H}_5\) (compd. no. 3) shows a decrease (0.922 eV) in the value of LUMO energy. Thus, ethyl-\(p\)-azoxybenzoate has lower value of LUMO energy than the former compounds. On further replacement of \(-\text{OCH}_3\) group by \(-\text{CH}═\text{CH}–\text{COOC}_2\text{H}_5\) (ethyl-\(p\)-azoxycinnamate) shows a decrease in the 2.058 eV and 2.108 eV value of LUMO energy with respect to compd. no. 1 and 2 but an increment of 0.026 in respect to 3. Finally, replacement of \(-\text{OCH}_3\) group by \(-\text{CH}═\text{CH}–\text{COOC}_8\text{H}_{17}\) (\(n\)-octyl-\(p\)-azoxyccinnamate) shows an abnormal decrease of 73.121 eV in the LUMO energy. The decreasing order of LUMO energy of above LCs for nucleophilic interaction shows trend similar to the HOMO energy, \(p\)-azoxyphenetole > \(p\)-azoxyanisole > ethyl-\(p\)-azoxyccinnamate > ethyl-\(p\)-azoxybenzoate > \(n\)-octyl-\(p\)-azoxyccinnamate (Figure 3).

### Table 4. Energy of lowest unoccupied molecular orbital of azoxy-based LC

| Compd. Name                  | \(\varepsilon\) LUMO (eV) |
|------------------------------|----------------------------|
| \(p\)-azoxyanisole           | -2.718                     |
| \(p\)-azoxyphenetole         | -2.668                     |
| ethyl-\(p\)-azoxybenzoate    | -3.640                     |
| ethyl-\(p\)-azoxyccinnamate  | -3.806                     |
| \(n\)-octyl-\(p\)-azoxyccinnamate | -78.115                    |

The HOMO-LUMO gap, i.e. the difference in energy between the HOMO and LUMO, is an important stability index [14]. A large HOMO-LUMO gap implies high stability for the molecule in the sense of its lower reactivity in chemical reactions. The HOMO-LUMO
gaps of the above LCs were calculated and are also reported in Table 5. A reference to the data shows the following sequence of above LCs with respect to their stability: Ethyl-\textit{p}-azoxycinnamate > \textit{p}-Azoxyphenetole > \textit{p}-Azoxyanisole > Ethyl-\textit{p}-azoxybenzoate > \textit{n}-Octyl-\textit{p}-azoxycinnamate. The trend of HOMO-LUMO gap is also demonstrated by Figure 4.

### Table 5. HOMO-LUMO energy gap of azoxy-based LC

| Compd. Name                | HOMO-LUMO gap |
|----------------------------|---------------|
| \textit{p}-azoxyanisole    | 2.276         |
| \textit{p}-azoxyphenetole  | 2.273         |
| ethyl-\textit{p}-azoxybenzoate | 2.323     |
| ethyl-\textit{p}-azoxycinnamate | 1.939    |
| \textit{n}-octyl-\textit{p}-azoxycinnamate | 2.583    |

![Figure 4](image)

**Figure 4.** Graph showing effect of substitution on HOMO-LUMO energy gap of the compound

### 3.3. Ionization Energy (IE)

The minimal energy needed for the detachment of an electron for an atom or a molecule [15]. According to Koopman’s theorem [16], the EA is simply the eigenvalue of HOMO with change in sign (IP = -\(\varepsilon\)HOMO) and characterizes the susceptibility of the molecule toward attack by electrophiles. The IP of the above LCs were calculated directly from the structure of the compound and are reported in Table 6. A reference to the table indicates that the IE of RC is 4.994. On replacement of –OCH\(_3\) group of RC by –OC\(_2\)H\(_5\), there is a decrease of 0.053 eV value of ionization energy of the resulted compound, \textit{p}-azoxyphenetole. Similarly, replacement of –OCH\(_3\) group by –COOC\(_2\)H\(_5\) (compd. no. 3) shows an increase (0.969 eV) in the value of ionization energy. Thus, ethyl-\textit{p}-azoxybenzoate has larger value of ionization energy of 1.022 eV than the former compounds. On further replacement of –OCH\(_3\) group by \textit{CH}=\textit{CH}–COOC\(_2\)H\(_5\) (ethyl-\textit{p}-azoxycinnamate) shows an increase in the value of ionization energy with respect to compd. no. 1 and 2 and decrease in respect to 3. Finally, replacement of –OCH\(_3\) group by \textit{CH}=\textit{CH}–COOC\(_2\)H\(_{17}\) (\textit{n}-octyl-\textit{p}-azoxycinnamate) shows an abnormal increase in the ionization energy. The increasing order of IE of above LCs shows trend opposite to the HOMO energy (IE = -\(\varepsilon\)HOMO), \textit{p}-azoxyphenetole > \textit{p}-azoxyanisole > ethyl-\textit{p}-azoxybenzoate > ethyl-\textit{p}-azoxybenzoate > \textit{n}-octyl-\textit{p}-azoxycinnamate and is good agreement to the Koopman’s theorem (Figure 5).

### Table 6. Ionisation energy of azoxy-based LC

| Compd. Name                | IE (eV)  |
|----------------------------|----------|
| \textit{p}-azoxyanisole    | 4.994    |
| \textit{p}-azoxyphenetole  | 4.941    |
| ethyl-\textit{p}-azoxybenzoate | 5.963   |
| ethyl-\textit{p}-azoxybenzoate | 5.745   |
| \textit{n}-octyl-\textit{p}-azoxycinnamate | 75.532  |
Figure 5. Graph showing effect of substitution on ionization potential of the compound

3.4. Electron Affinity (EA)

The energy difference between an uncharged species and its negative ion, referred to as an electron affinity, is an important property of atoms and molecules [15]. A survey of examples illustrates the diversity of areas in which electron affinities play a role: silicon and quantum dot (nanocrystal) semiconductor chemistry, Schottky diodes, molecular clusters, fullerene chemistry, interstellar chemistry, polymer photoluminescence, microelectronics, flat panel displays, and even hypotheses regarding the shuttle glow phenomenon. The EA of the above LCs were calculated directly from the structure of the compound and are reported in Table 7. A reference to this table indicates that the EA of RC is 2.718 eV. On replacement of –OCH₃ group of RC by –OC₂H₅, there is a decrease of 0.05 eV value of EA of p-azoxyphenetole. Similarly, replacement of –OCH₃ group by –COOC₂H₅ (compd. no. 3) shows a decrease (0.922 eV) in the value of EA. Thus, ethyl-p-azoxybenzoate has larger value of EA than the former compounds. On further replacement of –OCH₃ group by –CH=CH–COOC₂H₅ (n-octyl-p-azoxyccinnamate) shows an abnormal increase of 73.121 eV in the EA. The increasing order of EA of above LCs shows trend opposite to the LUMO energy (EA = –εLUMO), n-octyl-p-azoxyccinnamate > ethyl-p-azoxybenzoate > ethyl-p-azoxyccinnamate > p-azoxyanisole > p-azoxyphenetole (Figure 6). It is good agreement of the Koopman’s theorem, according to which the EA is simply the eigenvalue of LUMO with change in sign and characterizes the susceptibility of the molecule toward nucleophilic interaction.

Table 7. Electron affinity of azoxy-based LCs

| Compd. Name                      | EA (eV) |
|---------------------------------|---------|
| p-azoxyanisole                  | 2.718   |
| p-azoxyphenetole                | 2.668   |
| ethyl-p-azoxybenzoate           | 3.640   |
| ethyl-p-azoxyccinnamate         | 3.806   |
| n-octyl-p-azoxyccinnamate       | 78.115  |
3.5. Electronegativity ($\chi$)

In DFT, the electronegativity, commonly known to a chemist, is defined as the negative of a partial derivative of energy $E$ of an atomic or molecular system with respect to the number of electrons $N$ with a constant external potential $v(\textbf{r})$ [15].

$$\mu = -\chi = -(E/N)_{v(\textbf{r})}$$

When assuming a quadratic relationship between $E$ and $N$ a finite difference approximation Eq. 2 may be rewritten as

$$\chi = -\mu = -(IP + EA)/2$$

where IP and EA are the vertical ionization energy and electron affinity, respectively, thereby recovering the electronegativity definition of Mulliken [17]. Moreover, a theoretical justification was provided for Sanderson’s principle of electronegativity equalization, which states that when two or more atoms come together to form a molecule, their electronegativities become adjusted to the same intermediate value. According to Koopman’s theorem [16], the IP or IE is simply the eigenvalue of HOMO with change in sign and EA is the eigenvalue of LUMO with change of sign; hence Eq. 3 may be written as

$$\chi = -\mu = \frac{1}{2}(\varepsilon_{\text{LUMO}} + \varepsilon_{\text{HOMO}})$$

The $\chi$ of the above LCs were calculated by solving the Eq. 4 and are reported in Table 8. A reference to this table indicates that the $\chi$ of RC is -3.856 eV. On replacement of $-\text{OCH}_3$ group of RC by $-\text{OC}_2\text{H}_5$, there is an increase of 0.051 eV value of $\chi$ of the resulted compound, $p$-azoxyphenetole. Similarly, replacement of $-\text{OCH}_3$ group by $-\text{COOC}_2\text{H}_5$ (compd. no. 3) shows a decrease (0.946 eV) in the value of $\chi$. Thus, ethyl-$p$-azoxybenzoate has lower value of $\chi$ than the former compounds. On further replacement of $-\text{OCH}_3$ group by $-\text{CH}=-\text{CH}-\text{COOC}_2\text{H}_5$ (ethyl-$p$-azoxyccinnamate) shows a decrease in the 0.092 eV and 0.0971 eV value of $\chi$ with respect to compd. no. 1 and 2 but an increment of 0.026 in respect to 3. Finally, replacement of $-\text{OCH}_3$ group by $-\text{CH}=-\text{CH}-\text{COOC}_2\text{H}_5$: (n-octyl-$p$-azoxyccinnamate) shows an abnormal decrease of 72.968 eV in the $\chi$. The decreasing order of $\chi$ of above LCs is: $p$-azoxyphenetole > $p$-azoxyanisole > ethyl-$p$-azoxybenzoate > ethyl-$p$-azoxyccinnamate > n-octyl-$p$-azoxyccinnamate (Figure 7).

| Compd. Name          | $\chi$ (eV) |
|----------------------|-------------|
| $p$-azoxyanisole     | -3.856      |
| $p$-azoxyphenetole   | -3.805      |
| ethyl-$p$-azoxybenzoate | -4.802    |
| ethyl-$p$-azoxyccinnamate | -4.776  |
| n-octyl-$p$-azoxyccinnamate | -76.824 |

**Figure 6.** Graph showing effect of substitution on electron affinity of the compound

**Table 8.** Electronegativity of azoxy-based LC
3.6. Absolute hardness (\(\eta\))

The absolute hardness \(\eta\) is defined as

\[
\eta = \frac{1}{2} \left( \delta \mu / \delta N \right) v(r) = \frac{1}{2} \left( \delta^2 E / \delta N^2 \right) v(r)
\]  

(5)

where \(E\) is the total energy, \(N\) is the number of electrons of the chemical species, and \(v(r)\) is the external potential [15]. The operational definition of absolute hardness is given as

\[
\eta = \frac{1}{2} (\text{IP} + \text{EA})
\]  

(6)

where IP and EA are the vertical ionization energy and electron affinity, respectively, of the chemical species. According to Koopman’s theorem [16], the IP or IE is simply the eigenvalue of HOMO with change in sign and EA is the eigenvalue of LUMO with change of sign; hence Eq. 6 may be written as

\[
\eta = \frac{1}{2} (\epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}})
\]  

(7)

The \(\eta\) of the above LCs were calculated by solving the Eq. 7 and are reported in Table 9. A reference to this table indicates that the \(\eta\) of RC is 1.138 eV. On replacement of –OCH\(_3\) group of RC by –OC\(_2\)H\(_5\), there is a decrease of 0.001 eV value of \(\eta\) of the resulted compound, p-azoxyphenetole. Similarly, replacement of –OCH\(_3\) group by –COOC\(_2\)H\(_5\) (compd. no. 3) shows an increase of 0.024 eV in the value of \(\eta\). Thus, ethyl-p-azoxybenzoate has higher value of \(\eta\) than the former compounds. On further replacement of –OCH\(_3\) group by –CH=CH–COOC\(_2\)H\(_5\) (ethyl-p-azoxybenzoate) shows an increase of 0.168 eV, 0.167 eV and 0.192 eV in the value of \(\eta\) with respect to compd. no. 1, 2 and 3. Finally, replacement of –OCH\(_3\) group by –CH=CH–COOC\(_2\)H\(_17\) shows a negative value of \(\eta\), -1.292 eV. The decreasing order of \(\eta\) of above LCs is: ethyl-p-azoxybenzoate > p-azoxyanisole > p-azoxyphenetole > ethyl-p-azoxybenzoate > ethyl-p-azoxybenzylamine > n-octyl-p-azoxybenzylamine (Figure 8).

Table 9. Absolute hardness of azoxy-based LC

| Compd. Name             | \(\eta\) (eV) |
|-------------------------|---------------|
| p-azoxyanisole          | 1.138         |
| p-azoxyphenetole        | 1.137         |
| ethyl-p-azoxybenzoate   | 1.162         |
| ethyl-p-azoxybenzylamine| 0.970         |
| n-octyl-p-azoxybenzylamine| -1.292       |
3.7. Dipole moment ($\mu$)

The dipole moments of polyatomic molecules depend on the nature of the atoms and on their arrangement. The dipole moment of a molecule is the vector sum of the dipole moments of the bonds and is calculated according to the rule of vector addition [18]. If two bonds with the dipole moments $P$ and $Q$ are at an angle $\theta$ the total dipole moment is given by

$$\mu^2 = P^2 + Q^2 + 2PQ \cos \theta$$

(8)

For instance two identical bonds with the opposite directions ($\theta = 180^\circ$) have $\mu = 0$. For identical bonds ($P = Q$) Eq. 8 yields

$$\mu^2 = 2P^2 (1 + \cos \theta)$$

(9)

The dipole moments of the above LCs were computed directly from the optimized structure and are reported in Table 10. A reference to the data shows that the dipole moment of RC is 1.343 D. On replacement of $-OCH_3$ group of RC by $-OC_6H_5$ there is a decrease of 0.146 D of the resulted compound, $p$-azoxyphenetole. Further, replacement of $-OCH_3$ group of RC by $-COOC_2H_5$, $-CH=CH$-$COOC_2H_5$ and $-CH=CH$-$COOC_8H_{17}$ groups increases the dipole moments of the resulting compounds. This is also demonstrated by Figure 9.

**Table 10. Dipole moment of azoxy-based LC**

| No. | Compd. Name               | $\mu$ (D) |
|-----|----------------------------|-----------|
| 1   | $p$-azoxyanisole          | 1.343     |
| 2   | $p$-azoxyphenetole        | 1.197     |
| 3   | ethyl-$p$-azoxybenzoate   | 2.194     |
| 4   | ethyl-$p$-azoxyccinnamate | 5.332     |
| 5   | $n$-octyl-$p$-azoxyccinnamate | 6.070  |

**Figure 8.** Graph showing effect of substitution on absolute hardness of the compound

**Figure 9.** Graph showing effect of substitution on dipole moment of the compound
4. Conclusions

Above study concluded that
1. Total energy increases in sequence -OCH₃ < -OC₆H₅ < -COOC₆H₅ < -CH-COOC₆H₅ < -CH=CH-COOC₆H₅ showing the stability of LCs.
2. The decreasing order of HOMO energy of above LCs for electrophilic interaction is p-azoxyphenetole > p-azoxyanisole > ethyl-p-azoxybenzoate > n-octyl-p-azoxybenzoate.
3. The decreasing order of LUMO energy of above LCs for nucleophilic interaction shows trend similar to the HOMO energy.
4. The increasing order of IE of above LCs show trend opposite to the HOMO energy and the increasing order of EA of above LCs shows trend opposite to the LUMO energy that are good agreement to the Koopman’s theorem.
5. The decreasing order of χ of above LCs is: p-azoxyphenetole > p-azoxyanisole > ethyl-p-azoxybenzoate > n-octyl-p-azoxybenzoate.
6. The decreasing order of η of above LCs show trend similar to the χ.
7. The dipole moment increases in sequence -OCH₃ < -OC₆H₅ < -COOC₆H₅ < -CH=CH-COOC₆H₅ showing polar interaction behaviour.

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