Electro-optical properties of Liquid Crystal molecules by Quantum Mechanical methods

Summary of the

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Summary

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The liquid crystal is a state of matter which exists in a semisolid phase of nature. When a solid is going through the process of heating, it converts into liquid. But there exists also some solids which, when heated, convert into a turbid liquid. On further increasing the temperature of such solids, one converts turbid liquid to isotropic liquid. Such an intermediate phase between the crystalline solid and isotropic liquid is known as the liquid crystal phase [1-5]. The molecules of liquid crystal exhibit properties of solid as well as liquid. Liquid crystal molecule possesses orderly arrangement, optical activity like solidity and fluidity, viscosity, surface tension, etc. like liquid. They diffuse like the molecules in a liquid, but also maintain their orientation order along with positional order. The molecules in LC’s are pointing in a certain direction and certain position compared to others [6-12].

Liquid crystals are classified into the thermotropic liquid crystal which is obtained within a temperature range [13-15], and lyotropic liquid crystals which are obtained within concentration range [16-18]. Thermotropic liquid crystals are further classified into nematic, smectic, cholesteric liquid crystals depending upon the molecular symmetry and orientation of the molecules. The nematic liquid crystal is an anisotropic fluid and the molecules in the nematic are free to move in any direction as they don’t have an orderly position [5, 19].

Liquid crystals have properties depending upon the anisotropic nature of the molecules. The molecules of liquid crystal have the property of alignment in the direction of the external electric field. The order parameter of the liquid crystal is derived or calculated from the transition between different phases according to the breaking of symmetry. Order parameter describes a phase transition that must satisfy the requirements of $Q=0$ and $Q\neq0$ in the less ordered phase and the more ordered phase respectively [20-22].

The stability range of the liquid crystalline materials is defined by the difference in the transition temperature. The highly ordered phase exhibits the lower transition temperature in the polymorphic phase. For the homologous series of the liquid crystal compounds, the variations are observed for the given phase transition with an increasing number of alkyl or alkoxy chain length, the clearing point decreases. The odd-even effect is found in the liquid crystalline compound as the odd members of the chain length have lower clearing points.

The liquid crystals are very susceptible to an electric field regarding which the liquid crystal molecules are widely used in electro-optical applications or flat panel display devices based on their various molecular chemistry [23-26]. The optical anisotropy or birefringence is the physical property of the liquid crystal materials in which the materials possess various refractive indices in different directions. It is the property of alignment of the liquid crystals to control the polarization of the incident light which resulted in widespread display applications. The uniaxial behavior of the liquid crystals is known as the birefringent or doubly refractive which exists in two different refractive indices: the ordinary refractive index n_o and extraordinary refractive index n_e. The difference between these two principal refractive indices is used to calculate the birefringence of the liquid crystal. The value of birefringence for rod-like molecules is positive, i.e. $\Delta n>0$, and is negatively valued for the discotic molecules [27-31].

There is broad research on the theoretical approaches of these materials which gives us a lot of ambiguous results. [32-35].

The thesis present here is divided into six chapters which all are briefly described below:

Chapter 1 describes the "Introduction" of the liquid crystal molecules as liquid crystals exhibit the various properties of the crystalline solid and isotropic liquid. The molecular structure of liquid crystal consists of a side chain with a terminal group that interacts with aromatic rings, attached to linkage groups [36-40]. The liquid crystal is classified into different types based on molecular symmetry or arrangement of molecules.

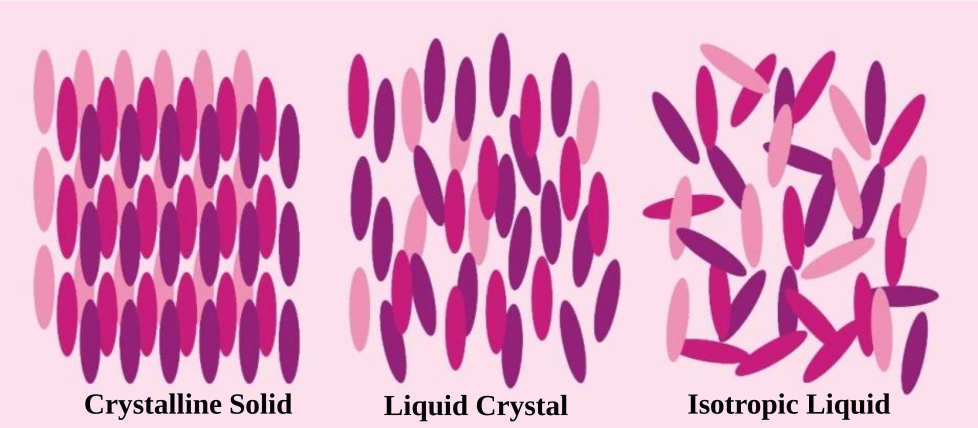

Figure 1. Molecular arrangements of Liquid crystal molecules.

The nematic phase of liquid crystal is the simplest form in which there is no orientational order and the molecules align themselves in the preferred direction. In smectic liquid crystals, molecules have positional as well as directional order and exhibit soap-like properties. Cholesteric LC's have long-chain chirality order in molecules and are structured in the helical form. These liquid crystals exhibit the property of diffraction of light [41].

The chapter also includes the physical properties of the liquid crystal-like optical anisotropy, dielectric anisotropy, elastic constants, viscosity, order parameter, etc.

On applying the electric field, the molecules of liquid crystal orient themselves in the direction of the field which is applied in a certain direction.

Liquid crystals are widely used in the discipline of technology, science, and also in medicine. They are used in display devices, optical imaging, medical science, and temperature sensors, etc. A brief introduction of applications like liquid crystal display (LCD), liquid crystal thermometer, and other applications are discussed in the chapter [41-43].

Chapter 2 gives the “Computational methodology” of the molecules to calculate the physical properties from the optimization of the liquid crystal. It starts from the computational Quantum mechanics in which we solve the minimum energy of the molecules from the density functional theory, method using the preferred basis set and the methods [44-46]. The main basis of DFT depends on the electron density, i.e. if the electron density is found, then other possible parameters are also calculated. The mathematical formulation of the physical properties like order parameter, birefringence, refractive index, the magic angle is derived which are described in the chapter. Gaussian 09 software [43, 47] is used for the designing and optimization of the molecules.

Chapter 3 gives the “Electro-optical odd-even effect of the APAPA liquid crystal molecule studied under the influence of an extraneous electric field (THz)”. The structure of the APAPA liquid crystal consists of two benzene rings that connect with the Schiff base linkage group. According to Mandal et.al. [48], the order parameter of the APAPA liquid crystal lies between 0.61 to 0.40. In the given chapter, an electric field in the range from 0.0000 (a.u.) to 0.1000 (a.u.) is applied to the homologous series of the APAPA liquid crystal after the optimization of the molecules from the Gaussian 09 software [49] B3LYP [50-53] and M062X [52] methods using 6-31G** basis sets [53-54]. Ordinary molecular polarizability (α_o), and extraordinary molecular polarizability (α_e) are calculated after applying an electric field to the molecular series after which the order parameter, refractive index, birefringence, the magic angle is calculated from the given equations in the chapter. In the present work, B3LYP and M062X both methods are used for comparing the results. The birefringence of the APAPA liquid crystal series gives an odd-even effect on increasing the alkyl chain length under the effect of an electric field. Both methods give similar results.

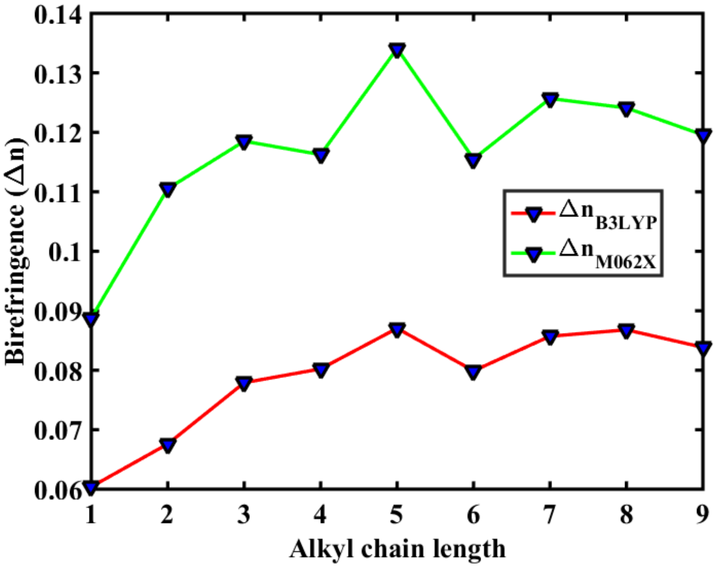

Figure 2. Odd-even effect of birefringence calculated under the influence of an electric field.

The order parameter is calculated from the equation given in the chapter under the impact of an electric field. The value of the order parameter of 1MBA is -0.54 and for 3MBA, -0.68 is calculated, which results from the negative order parameter and is shown in the following Figure 3.

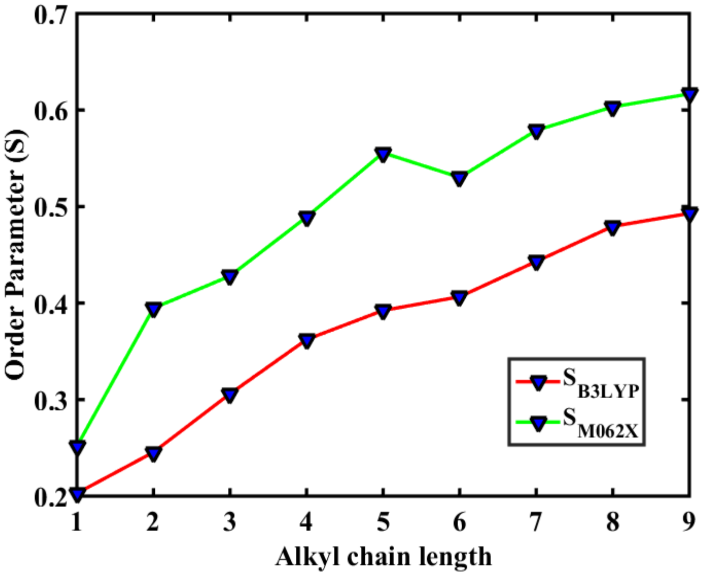

Figure 3. The order parameter of the homologous series continually increases with an extension of the alkyl chain length.

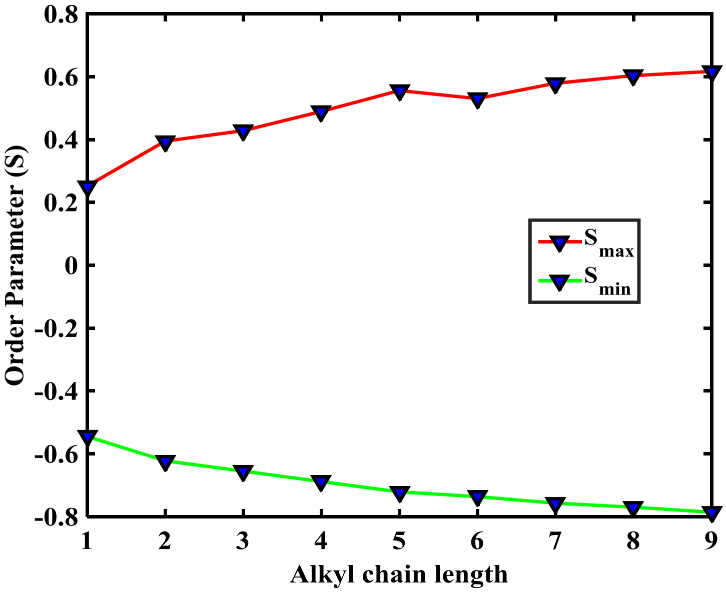

Figure 4. Positive as well as negative order parameters were calculated under the influence of an extraneous electric field in THz frequency.

The director angle (θ=90) of the APAPA liquid crystal remains constant for the whole molecular series as shown in Figure 5. It is derived from the equation given in the chapter by the electric field in the THz frequency.

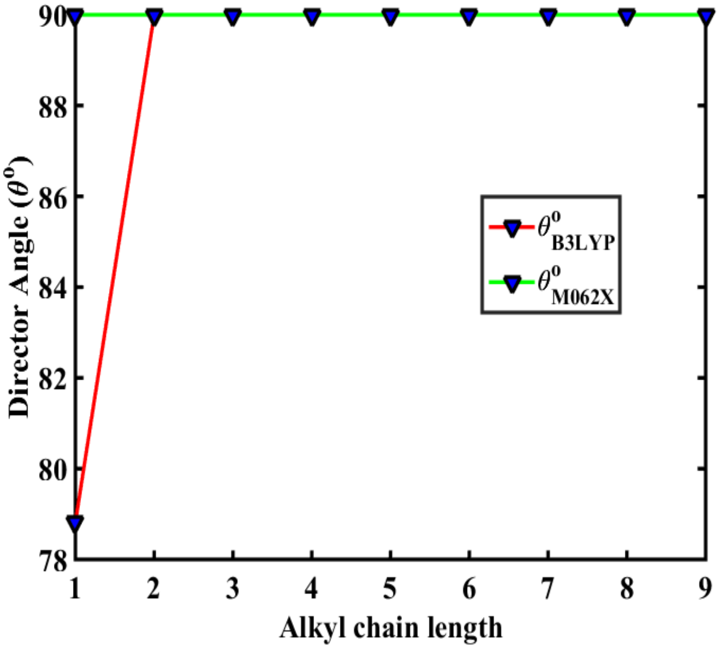

Figure 5. Director angle remains constant of the homologous series under the influence of the electric field.

The dipole moment of the homologous series of APAPA liquid crystal molecules continuously decreases with increasing the alkyl chain length as shown in Figure 6. This is the reason due to which the higher range of homologous series is not convenient for the use in liquid crystal characteristics.

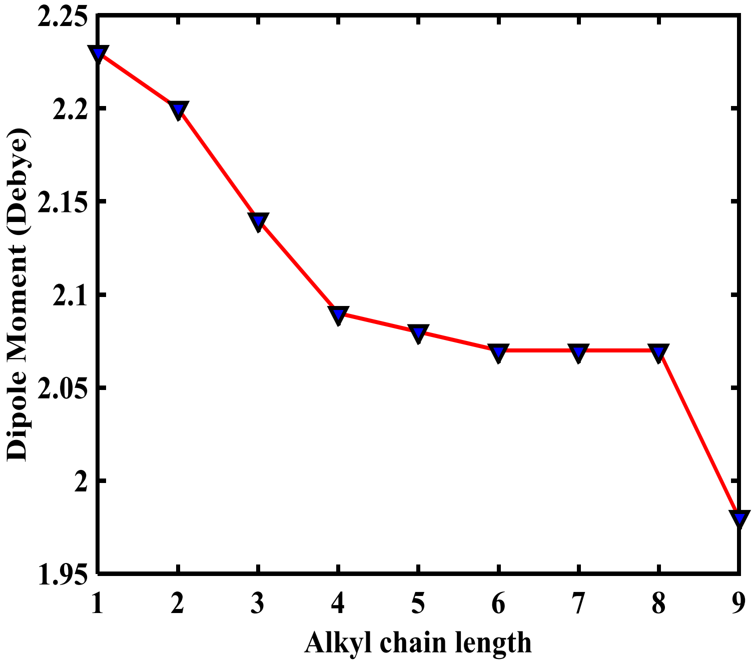

Figure 6. The dipole moment of the homologous series is calculated with an extension on the alkyl chain length.

Hence, with an expansion of alkyl chain length, the homologous series shows the odd-even effect under the influence of the electric field. The birefringence, electron affinity, ionization potential exhibit the odd-even effect while the order parameter and refractive index do not show the odd-even effect. The given liquid crystal series is hence used for the photo luminance, sensing, scattering, and THz application devices.

Chapter 4 describes the "Electro-optical parameters with adverse order of 10CB liquid crystal molecule studied under the influence of an external high electric field". Cyano biphenyl liquid crystals are used in electro-optical display devices from being the most stable compound. The value of bandgap is found higher in the higher homologous series of molecules as they construct the more planar structure. In the present chapter, 10CB liquid crystal molecule is optimized by Gaussian 09 software [49] using the density functional theory method B3LYP [50-53]. An electric field is applied along the molecular (x-axis) and perpendicular (y-axis) to the molecular axis, to the molecule after the optimization. The electro-optical properties of the 10CB liquid crystal molecule are calculated from the mathematical equations given in the chapter. The order parameter of the 10CB liquid crystal is 0.63 which is positive and -0.40 is the negative value as shown in Figure 7.

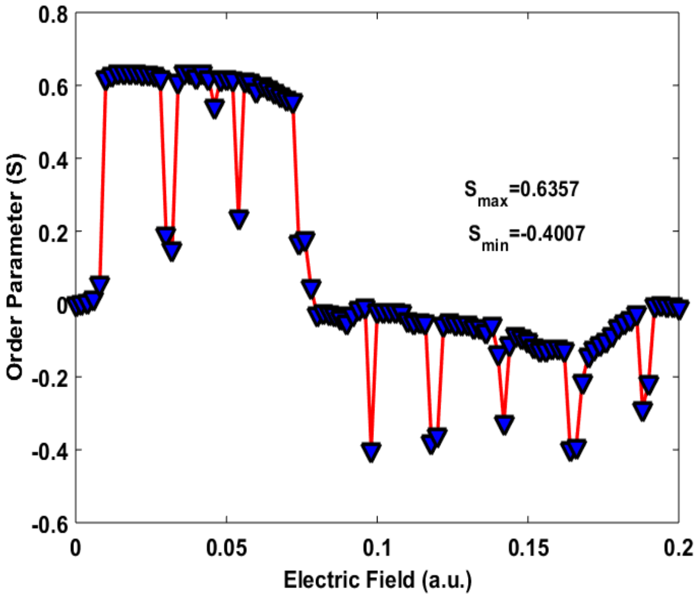

Figure 7. The order parameter of 10 CB liquid crystals under the influence of the electric field

The molecules exhibit a three-phase transition as a smectic-nematic-isotropic phase under an electric field. At the isotropic phase, 10CB molecules gain stability. The director angle is found stable for the smectic A phase. The maximum range is 75.09 degrees and the minimum range is 29.52 degrees is calculated for the director angle of 10CB.

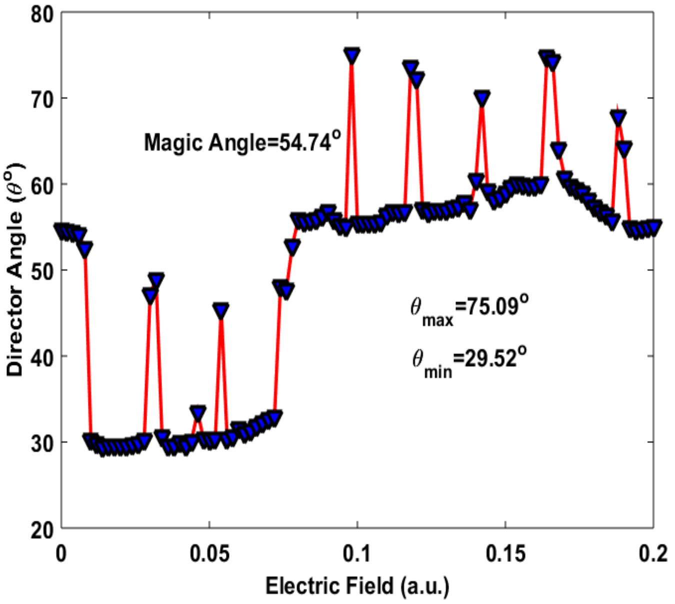

Figure 8. Director Angle of 10CB liquid crystal under the influence of an electric field

The birefringence of the 10CB liquid crystal compound is shown in Figure 9.

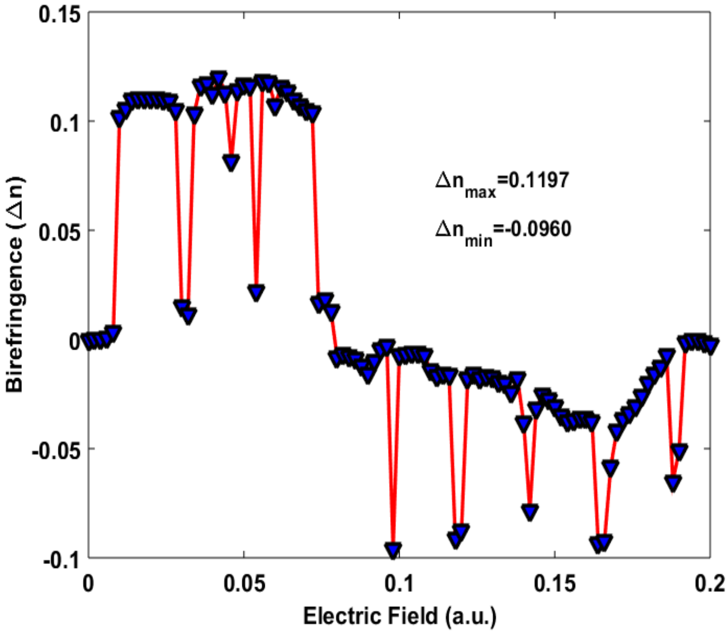

Figure 9. Birefringence of 10CB liquid crystal. (The maximum birefringence of 10CB LC is Δn=0.1197 and the minimum birefringence is Δn=-0.0960).

The chapter concluded that the 10CB molecule shows the value of the negative order parameter in the range of high electric fields. Due to this, the bandgap of the molecule decreases for the positive order parameter and increases for the negative order parameter. Also for the higher member of the homologous series, 10CB expresses a large bandgap of the range 3.60 eV. The bandgap of the compound is affected by the applied electric field. So the LC's are used as tunable bandgap applications. The order parameter affects the electro-optical properties in liquid crystals.

Chapter 5 describes the "Comparative DFT study of parallel and antiparallel conformation of 5CB and 6CB liquid crystal dimers". In 5CB and 6CB liquid crystals, the molecular structure contains conjugated rigid cores in long-range. With the cyano group, the molecule exhibit higher birefringence [54-56]. In the present chapter, 5CB and 6CB molecules are optimized with NWChem software [57] with the density functional theory method. Here 360 conformations are generated in which only 4 conformations of minimum energies are used for interaction with each other. After interaction in different conformations, the molecular properties of the 5CB, 6CB dimers have been calculated with the LC-BLYP method.

At first, we calculated interaction properties of the 5CB-5CB dimer in the parallel conformation as in Figure 10.

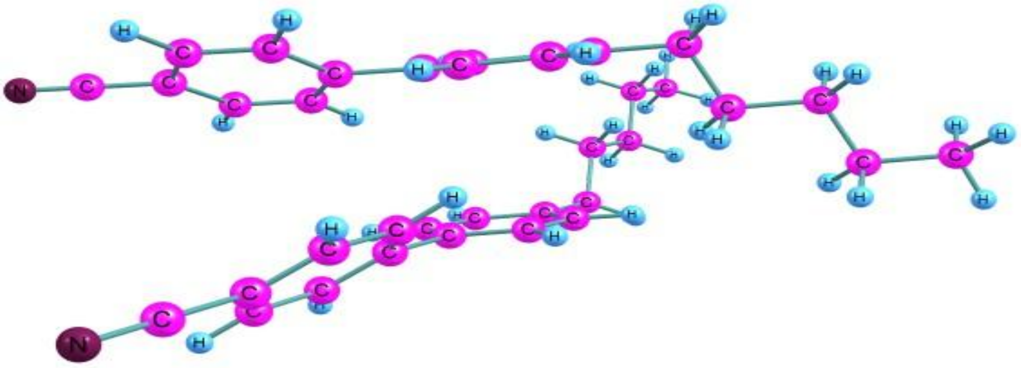

Figure 10. Parallel conformation of 5CB liquid crystal dimer.

In parallel conformation, one dimer of 5CB is kept stable and the second dimer of 5CB is moving in the forward or backward direction. Hence the properties found are tabulated in the following Table:

Table 1. The molecular properties of the 5CB-5CB dimer with parallel conformation at different positions in the forward direction.

5CB-5CB Parallel conformation	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.50	4.51	4.51	4.52	4.52
Dipole moment *(Debye)*	10.37	10.36	10.36	10.35	10.34
Thermal Energy *(kcal/Mol)*	427.71	427.69	427.08	427.07	427.68
Polarizability *(kcal/Mol)*	256867	256779	256691	256603	256522
Total Energy *(kcal/Mol)*	-9440.86	-9440.91	-9440.95	-9440.99	-9441.02
Heat capacity (CV) *(kcal/Mol)*	0.14	0.14	0.13	0.13	0.14
Entropy *(kcal/Mol)*	0.23	0.23	0.22	0.22	0.23
ZPE *(kcal/Mol)*	404.53	404.50	404.44	404.43	404.46
Enthalpy *(kcal/Mol)*	428.29	428.28	427.66	427.66	428.27
Gibbs Energy *(kcal/Mol)*	358.39	357.92	360.19	360.06	358.19

Table 2. The molecular properties of the 5CB-5CB dimer with parallel conformation at a different position in the backward direction.

5CB-5CB Parallel conformation	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.51	4.51	4.50	4.49	4.48
Dipole moment *(Debye)*	10.35	10.34	10.34	10.35	10.35
Thermal Energy*(kcal/mol)*	427.68	427.69	427.72	427.74	427.74
Polarizability*(kcal/mol)*	256377	256308	256239	256183	256120
Total Energy *(kcal/mol)*	-9440.06	-9440.07	-9440.07	-9440.07	-9440.06
Heat capacity (C_v)*(kcal/mol)*	0.14	0.14	0.14	0.14	0.14
Entropy *(kcal/mol)*	0.23	0.24	0.23	0.23	0.22
ZPE*(kcal/mol)*	404.46	404.46	404.50	404.54	404.53
Enthalpy *(kcal/mol)*	428.27	428.28	428.30	428.33	428.33
Gibbs Energy *(kcal/mol)*	358.11	357.89	358.25	358.43	358.16

In the antiparallel conformation of 5CB-5CB dimers, the molecular properties in the forward direction are given according to Table 3.

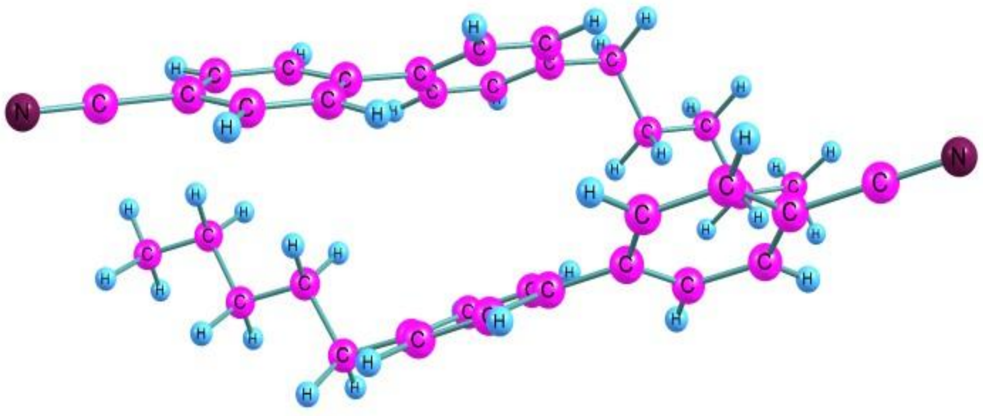

Figure 11. 5CB liquid crystal dimer in antiparallel conformation.

Table 3. The molecular properties of the 5CB-5CB dimer with antiparallel conformation at a different position in the forward direction.

5CB-5CB Antiparallel conformation	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.53	4.53	4.53	4.53	4.53
Dipole moment *(Debye)*	4.69	4.70	4.72	4.73	4.74
Thermal Energy *(kcal/Mol)*	427.66	427.66	427.65	427.64	427.63
Polarizability *(kcal/Mol)*	256478	256346	256227	256107	255994
Total Energy *(kcal/Mol)*	-9440.10	-9440.20	-9440.30	-9440.30	-9440.40
Heat capacity (CV) *(kcal/Mol)*	0.14	0.14	0.14	0.14	0.14
Entropy *(kcal/Mol)*	0.23	0.23	0.23	0.23	0.23
ZPE *(kcal/Mol)*	404.43	404.42	404.67	404.39	404.36
Enthalpy *(kcal/Mol)*	428.25	428.24	428.24	428.23	428.21
Gibbs Energy *(kcal/Mol)*	358.44	358.33	358.36	358.27	357.94

Table 4. The molecular properties of the 5CB-5CB dimer with antiparallel conformation at a different position in the backward direction.

5CB-5CB Antiparallel conformation	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.53	4.53	4.53	4.53	4.54
Dipole moment *(Debye)*	4.76	4.76	4.77	4.78	4.78
Thermal Energy*(kcal/mol)*	427.59	427.59	427.59	427.60	427.61
Polarizability*(kcal/mol)*	255794	255699	255612	255536	255474
Total Energy *(kcal/mol)*	-9440.30	-9440.40	-9440.50	-9440.60	-9440.70
Heat capacity (C_v) *(kcal/mol)*	0.14	0.14	0.14	0.14	0.14

Entropy *(kcal/mol)*	0.23	0.23	0.23	0.23	0.23
ZPE*(kcal/mol)*	404.29	404.27	404.27	404.29	404.30
Enthalpy *(kcal/mol)*	428.18	428.17	428.18	428.19	428.19
Gibbs Energy *(kcal/mol)*	357.27	357.25	357.23	357.36	357.43

The interaction properties of 5CB-5CB dimer in cross conformation are calculated which are shown in Table 5 in the forward direction:

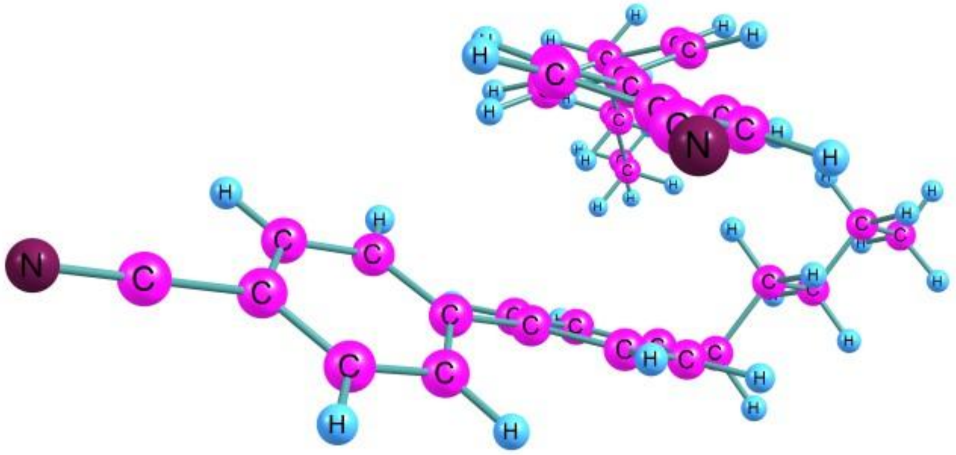

Figure 12. Cross conformation of 5CB liquid crystal dimer.

Table 5. The molecular properties of the 5CB-5CB dimer with cross conformation at a different position in a forward direction.

5CB-5CB **Cross conformation**	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.51	4.51	4.52	4.52	4.52
Dipole moment *(Debye)*	10.47	10.48	10.49	10.49	10.49
Thermal Energy *(kcal/Mol)*	427.61	427.00	426.98	426.98	427.56
Polarizability *(kcal/Mol)*	256089	255963	255844	255731	255630
Total Energy *(kcal/Mol)*	-9440.40	-9440.30	-9440.20	-9440.10	-9440.00

Heat capacity (CV) *(kcal/Mol)*	0.14	0.13	0.13	0.13	0.14
Entropy *(kcal/Mol)*	0.23	0.22	0.22	0.22	0.23
ZPE *(kcal/Mol)*	404.38	404.34	404.33	404.32	404.31
Enthalpy *(kcal/Mol)*	428.19	427.58	427.57	427.56	428.15
Gibbs Energy *(kcal/Mol)*	358.09	360.02	359.93	359.87	357.49

Table 6. The molecular properties of the 5CB-5CB dimer in cross conformation at a different position in the backward direction.

5CB-5CB Cross conformation	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.51	4.51	4.51	4.51	4.51
Dipole moment *(Debye)*	10.50	10.50	10.51	10.51	10.52
Thermal Energy*(kcal/mol)*	423.97	426.96	426.96	427.56	427.56
Polarizability*(kcal/mol)*	255436	255348	255267	255197	255122
Total Energy *(kcal/mol)*	-9440.10	-9440.08	-9440.06	-9440.05	-9440.03
Heat capacity (C_v) *(kcal/mol)*	0.13	0.13	0.13	0.14	0.14
Entropy *(kcal/mol)*	0.22	0.22	0.22	0.23	0.23
ZPE*(kcal/mol)*	404.29	404.27	404.27	404.28	404.28
Enthalpy *(kcal/mol)*	427.55	427.55	427.55	428.14	428.14
Gibbs Energy *(kcal/mol)*	359.67	359.56	359.48	353.21	357.10

The interaction properties of 6CB-6CB dimer in parallel conformation are calculated which are shown in Table 7 in the forward direction:

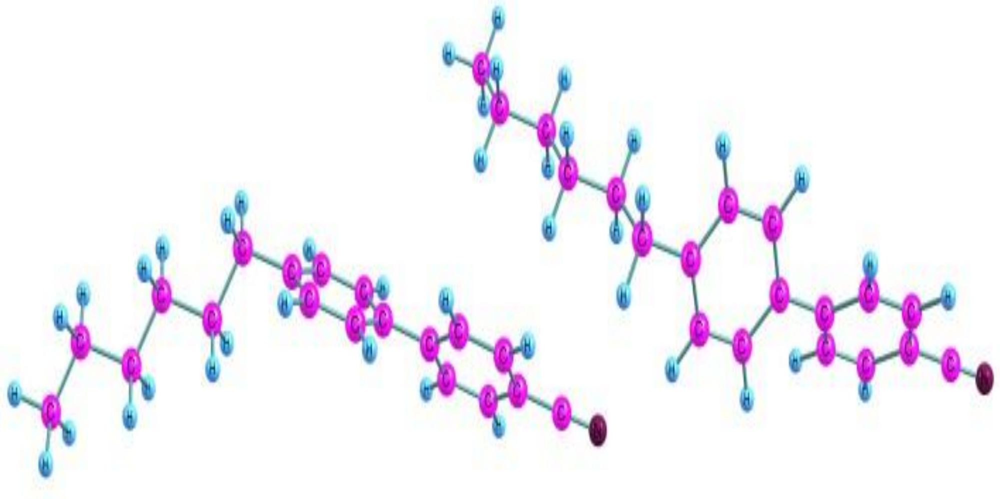

Figure 13. 6CB liquid crystal dimer in parallel conformation.

Table 7. The molecular properties of the 6CB-6CB dimer with parallel conformation at a different position in the forward direction.

6CB-6CB Parallel conformation	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.63	4.63	4.63	4.63	4.63
Dipole moment *(Debye)*	10.43	10.42	10.41	10.40	10.39
Thermal Energy*(kcal/mol)*	465.08	465.08	465.08	465.09	465.09
Polarizability*(kcal/mol)*	272065	272203	272341	272479	272623
Total Energy *(kcal/mol)*	-9933.32	-9933.38	-9933.43	-9933.48	-9933.54
Heat capacity (C_v) *(kcal/mol)*	0.15	0.15	0.15	0.15	0.15
Entropy *(kcal/mol)*	0.25	0.25	0.25	0.25	0.25
ZPE*(kcal/mol)*	440.16	440.16	440.17	440.16	440.17
Enthalpy *(kcal/mol)*	465.67	465.67	465.67	465.67	465.67
Gibbs Energy *(kcal/mol)*	390.70	390.76	390.76	390.43	390.55

Table 8. The molecular properties of the 6CB-6CB dimer with parallel conformation at a different position in the backward direction.

6CB-6CB **Parallel conformation**	**0.5Å**	**1.0Å**	**1.5Å**	**2.0Å**	**2.5Å**
HOMO-LUMO*(eV)*	4.64	4.64	4.64	4.64	4.64
Dipole moment *(Debye)*	10.38	10.37	10.37	10.36	10.35
Thermal Energy*(kcal/mol)*	464.49	464.48	464.48	464.49	464.49
Polarizability*(kcal/mol)*	272912	273056	273207	273351	273495
Total Energy *(kcal/mol)*	-9933.60	-9933.70	-9933.70	-9933.80	-9933.90
Heat capacity (C_v) *(kcal/mol)*	0.14	0.14	0.14	0.14	0.14
Entropy *(kcal/mol)*	0.24	0.24	0.24	0.24	0.24
ZPE*(kcal/mol)*	440.15	440.14	440.13	440.14	440.15
Enthalpy *(kcal/mol)*	465.07	465.07	465.07	465.07	465.08
Gibbs Energy *(kcal/mol)*	392.95	392.90	392.91	392.92	392.92

Hence we calculated all the interaction properties of 5CB-6CB and 6CB-6CB liquid crystal dimers in the parallel, antiparallel, and cross conformations with forwarding or backward directions which are described in the present chapter.

From the chapter, it has been concluded that the 5CB dimer in parallel conformations has high polarizability in comparison to others, and in 5CB-6CB antiparallel conformation, the smallest value of dipole moment with the smallest value of negative interaction energy is calculated. In the 6CB-6CB liquid crystal dimer in antiparallel conformation, the small value of isotropic polarizability is found and in the parallel conformation of 6CB dimer, the value of isotropic polarizability is found maximum.

Chapter 6 describes the conclusion and relative future prospects of the work presented in the thesis. By evaluating the transition temperature of the compounds, many LC's deviates from the magnitude of the order parameter. The electro-optical properties of the liquid crystal compounds are calculated by applying the electric field of the higher range.

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LIST OF PUBLICATIONS

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