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Physical, Electro-Optical, and Spectroscopic Properties of I52 Liquid Crystal: A Computational Study

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ABSTRACT

We have investigated the intrinsic molecular-level electronic, spectroscopic, and electric-field-dependent properties of 4-Ethyl-2-fluoro-4'-[2-(trans-4-pentylcyclohexyl)-ethyl] biphenyl (which is known as I52) using hybrid functional B3LYP with 6-31G basis set within Density Functional Theory (DFT) method. Dipole moment of I52 increases linearly with external electric field. UV spectra of I52 shows a sharp peak at 258 nm. Raman Spectra reveals C-H bonding (2800-3000cm $^{-1}$) is due to substituted ethyl and pentyl-cyclohexyl groups. FTIR spectra reveals C-H stretching vibrations at 3028 cm^{-1} due to alkyl side chains and trans-configuration of the pentyl-cyclohexyl moiety. HOMO-LUMO energy gap is found to be 5.08 eV, which makes I52 suitable for insulating applications. Structurally, I52 has a biphenyl core carrying an ethyl group and a fluorine atom on one phenyl ring and a large trans-4-pentylcyclohexylethyl substituent on the other, which is producing unique molecular anisotropy. The fluorine atom improved the dielectric anisotropy, which also leads to higher electro-optic effect. Hence, I52 continues to be a vital material in the study of fundamental liquid crystal science as well as in the application areas where customized molecular properties and good electro-optical performance are essential.

1. Introduction

4 - ethyl - 2 - fluoro - 4' - [2 - (trans - 4 - pentylcyclohexyl) - ethyl] - biphenyl, for short it's I52, is part of a group of compounds which have a low molecular mass mesogen structure and are widely used in nematic liquid crystal research because of their excellent physical and electro-optical properties. The molecular architecture of I52 combines several important structural types including the presence of a biphenyl core which provides rigidity and high aspect ratio, a fluoro substituent at the 2-position and an ethyl group at the 4-position present on one of the phenyl rings, contributing to the high molecular polarity and high thermal stability [1]. The other phenyl ring is substituted para with a unique ethyl chain with a trans-4-pentylcyclohexyl unit. The cyclohexyl ring is in the trans conformation, which is mainly, and provides linearity and reduces conformational disorder for efficient packing in the nematic phase. This specificity in molecular design gives I52 a very selective kind of flexibility and rigidity, which is needed on tuning the nematic phase width, dielectric anisotropy, and viscosity in liquid crystal mixtures [2].

From a synthetic point of view, I52 represents the new ways of approach used for advanced building blocks of liquid crystals. Its synthesis typically relies on such coupling reactions as Suzuki or Wittig cross-couplings where the synthesis starts with the preparation of functionalized biphenyl intermediates with fluoro and alkyl substituents. The ethyl linkage allows the tethering of bulky cyclohexyl derivatives, which is usually done by Grignard, Friedel-

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Crafts or palladium-catalysed reactions [3-5]. The trans-4-pentylcyclohexyl fragment plays an important role: the large steric bulk of the trans-4-pentylcyclohexyl group induces lateral interactions and reduces the rotational freedom, which have an effect on the smectic clustering and nematic phase stabilization [6]. The synthetic route is optimized to keep the purity of this high, often with performing strict chromatographic separation, as it is known that trace impurities in liquid crystal hosts have a dramatic effect on the phase behaviour and device reliability.

The physical characteristics of the I52 established a standard in terms of nematic liquid crystal host media particularly those that are used in displays and optical modulators [7, 8]. I52 is a compound with a high clearing point (usually above 80^{o}C), medium viscosity, and large positive dielectric anisotropy, which are required for fast switching and low voltage driving in LCD versions. The biphenyl structure is necessary to guarantee a high order parameter and high birefringence and the cyclohexyl moiety enhances compatibility with a variety of other nematic and smectic components utilized in device-grade blends [9]. Its distinctive mix of fluoro and alkyl constituency customizes a dosage of dipole moment and polarizability, decidingly furthermore crucial for processability in skinny cells and also earn steady electric field charge and electrical alignment. In the case of practical mixtures, I52 is mixed with other compounds (such as cyanobiphenyls and phenylcyclohexanes) to fine-tune the temperature ranges, viscosity and clearing points to fit device specifications [10-12].

Applications of I52, both span laboratory and industrial realms, fall in the versatility of I52. In research, I52 is very popular for studies of anisotropic interactions, pattern formation, and electroconvection in nematic phases due to its outstanding physical clearness and reproducibility. Its clearly outlined phase behavior is useful in precision calibration of differential scanning calorimeter (DSC) and cell alignment instructions in optical cells. I52 is used as a nematic dopant in commercial devices as well as dopant in a multi-component system used in active-matrix liquid crystal displays (AMLCDs), spatial light modulators, and optoelectronic switches [13]. Its good nematic phase and faster response time makes it suitable in a situation where image retention and dynamic contrast needs are minimal. Its dielectric anisotropy and high elastic constants are exploited to implement a high-performance, low-power, and long-life cycle of voltage-controllable retarders, phase shifters, and light shutters that can be engineered by device engineers [14].

I52 has still a complicated structure-property relations elucidated by theoretical and computational studies. First-principles predictions and molecular dynamics modelling of long-range nematic order and elastic properties shows that the interaction among biphenyl torsion, cyclohexyl orientation, and fluoro-alkyl topology of substitutes is what determines long-range nematic order [15-18]. Density Functional Theory (DFT) calculations show the remarkably high localization of electronic density all along the biphenyl backbone with stabilization effect of the end substituents and verified the preferred alignment in external magnetic and electric fields because of exacerbated molecule anisotropy. The conformer of the cyclohexyl unit is trans which maximizes the entropic values and takes parallel orientation in nematic domains. Advanced simulation protocols with I52 as a fodder molecule are applicable for the parameterization of intermolecular potentials, e.g. Gay-Berne potential, Maier-Saupe potential, parameterization and benchmarking of model failures in modelling of phase transitions, defects and electroconvection patterns. Such results help experimentalists in the design of liquid crystal hosts to support emergent photonic devices and displays of the next generation [19-21].

Experimental discoveries of I52 provide remarkable textures and phenomena, especially in the fields of electrohydrodynamic instabilities and pattern supply in fields applied. Studies have reported a wide variety of electroconvection structures, from Williams domains to oblique, zigzag, and chevron structures, which can be related to the strong coupling between director reorganisation and charge transport in the nematic phase [22,23]. The molecular uniformity of the compound enables low threshold voltage as well as sharp phase boundaries, important for adjusting the switching speeds and contrast ratios. The mechanisms of biphenyl torsion, polarization of fluoro-substituents, and cyclohexyl ring breathing are clarified by spectroscopic measurements (Raman, IR, UV). These data are key to verifying purity, orientation, and intermolecular interaction strength for liquid crystal cells manufactured for device benchmarking and calibration purposes [24-27].

I52 is still a milestone molecule in academic and industrial activities concerning the design of highly efficient liquid crystal hosts. Its remarkable molecular blueprint captures the choices of decades of liquid crystal chemistry combining gate way units with high order, fluid-like swimming polymer by use of flexible linkers, polar substituents with dielectric response, and bulky fragments with phase stability. With the ever-evolving nature of display technology toward higher-speed and brightness, as well as a reduced power consumption platform, molecules similar to I52 will find themselves playing a direct role to act as the templates of new generations of nematic and smectic materials [28].

In present study, we shall investigate the electronic, opto-electronic, thermo-dynamical, and spectroscopic properties of the I52 liquid crystal under the external electric field. In summary, 4-ethyl-2-fluoro-4'-[2-(trans-4-pentylcyclohexyl)-ethyl] biphenyl (I52) is a unique model compound with the combination of rigid aromatic and bulky cyclohexyl structures, fluoro and alkyl structures, and designed molecular polarity. Its preparation, phase behaviour, mechanical use, and computer modelling represent a vibrant field to materials scientists and engineers, in the field of developing and interpreting more complicated materials concerning liquid crystal technology.

2. Computational Methodology

We have used the NWChem software with hybrid functional (B3LYP) consists of a number of crucial steps [29, 30]. To start with, the molecular structure of I52 is optimised using B3LYP functional and 6-31G basis set. This choice reflects a balance between computational cost and

reliability for relatively large, π-conjugated and moderately polarizable organic systems. The geometry section specifies the atomic coordinates and the basis set section indicates the basis selected as 6-31G to be used at each atom in the molecule [31]. We performed the SCF convergence for stability check and geometry optimizations for the energy minimum structure, which is most suitable for further study [32]. After the optimization of the I52, an external electric field was applied along the x-axis (i.e long axis) of the molecule ranges from 0.00 a.u. to 0.10 a.u. [33]. These high field strengths do not represent typical macroscopic device conditions but are employed as a computational probe to systematically investigate molecular polarization response and electronic redistribution under strong perturbation. Dipole moment, polarizability, birefringence, etc. are calculated under external electric field. Furthermore, spectroscopic properties (FTIR, Raman, UV-Visible) were analysed. Molecular Orbital Energy (MOE) analysis was done to study the orbitals energy of I52.

3. Results and Discussion

Fig. 1 represents the optimised geometry of I52 liquid crystal. The I52 liquid crystal possesses normal anisotropic properties for thermotropic liquid crystals. Investigations show distinct phase transitions in I52 which can be explained in terms of its molecular structure which is presumably of rod-like (calamitic) character leading to promotion of the nematic phase at appropriate temperatures. Experimental measurements, often through methods like polarized optical microscopy or differential scanning calorimetry, show that there is a specific change from the isotropic liquid into birefringent nematic, which is marked bright domains behind crossed polarizers. The birefringence of the material, i.e. the difference between the extraordinary and ordinary refractive indices, provides confirmation of the orientational order that is so typical of the nematic phases.

Considering thermodynamic and optical studies, it appears that within the uniaxial nematic phase of I52, only the long axis orientational order is established and the centers of the molecular mass distribution are isotropic. This results in direction-dependent physical properties - most commonly in the dielectric constant, refractive index, and viscosity - the features that are also characteristics of liquid crystalline behaviour. Furthermore, any bulk deformation in the nematic phase can be described as a combination of splay, twist, and bend elastic deformations associated with the effective elastic constants. I52 reacts strongly to exogenous electric and magnetic fields where it re-aligns the director causing optical and dielectric properties to be modulated in a controlled manner, thus this material can be used in electro-optical applications.

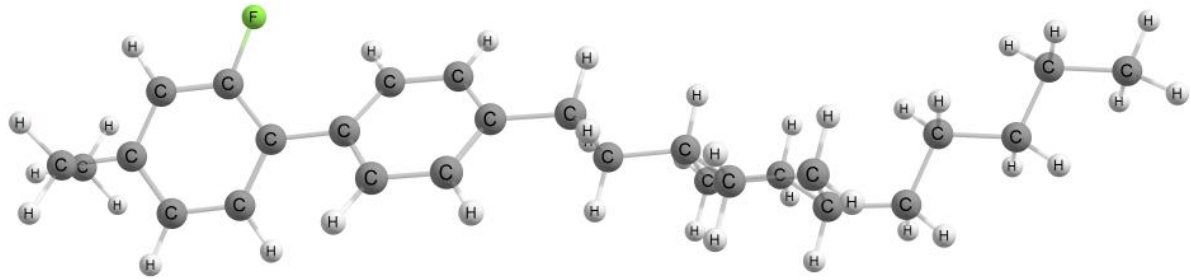

Fig. 1. Optimised geometry of I52 liquid crystal.

3.1. Electric-Field-Dependent Analysis of Electronic and Opto-Electronic Properties

3.1.1. Dipole Moment

Dipole moment is the key parameter to understand the molecular polarizability of a molecule. Generally, dipole moment increases with external electric field due to field effect. This trend can be seen in I52 LC as shown in Figure 2. The plot of dipole moment as a function of increasing electric field from 0.00 to 0.10 a.u. shows a drastic increase of dipole moment from negligible to higher than 800 Debye in value, which shows a strong polarization effect on the system studied here. At very low fields, however, dipole moment doesn't change because of weak interaction, and at intermediate and high fields it exhibits a nearly linear rise, indicating that the molecule has a high polarizability.

3.1.2. Polarizability

Polarizability play a vital role to investigate the opto-electronic properties of a liquid crystal molecule. Polarizability is sensitive to external stimuli like temperature or electric field. Figure 3 shows the variation in polarizability with external electric field of I52 liquid crystal molecule. At the beginning due to very weak external electric field, dipole moment doesn't change much and correspondingly polarizability remains almost same. But as the external electric field increases from 0.00 to 0.01 a.u., polarizability increases from 300 a.u. to 1500 a.u. Further increment in external electric field, changes the polarizability in small amount from 1500 a.u. to 1600 a.u. At external electric field 0.03 a.u., polarizability decreases to 500 a.u. This decrease in polarizability is due to re-entrant in nematic phase of the liquid crystal molecule. At odd number of external electric field, liquid crystal molecule re-entrant in the nematic phase which shows that I52 liquid crystal molecule is sensitive to external electric field.

3.1.3. Director Angle

Fig. 4 represents the variation in director angle (θ), also known as magic angle, of I52 liquid crystal as a function of applied electric field strength. The figure shows a characteristic Fredericks transition behaviour typical in electro-optical studies. Red lines represent simulated data points, forming sharp peaks that increase linearly from

about 30° at low fields (0.01–0.03 a.u.) to a maximum of θ_{max} = 54.7° near 0.06 a.u., before slight decrement. This graph represents the reorientation of liquid crystal molecules under an electric field, with the director angle saturating at higher fields (up to 50° on the y-axis scale). In our study, director angle found to be θ_{max} = 54.7° which matches with the reference magic angle (54.73°), likely indicating optimal alignment for spectroscopic or dielectric measurements in nematic phases.

3.1.4. Refractive Index

Refractive index of a liquid crystal material plays vital role in designing the opto-electronic devices with required properties. Figure 5 shows the refractive index (n) of I52 liquid crystal material as a function of applied electric field, capturing field-induced birefringence changes post-Fredericks transition. Graph of refractive index shows n ≈ 1.5735 at zero field, rising sharply to n ≈ 1.58 by 0.03 a.u., then oscillating slightly around 1.577–1.58 up to 0.1 a.u. From the graph, average refractive index is found to be n ≈ 1.577, at higher fields where director alignment stabilizes. This behaviour aligns with electro-optical modulation in nematic liquid crystals, where refractive index shifts due to molecular arrangement.

3.1.5. Birefringence

Fig. 6 represents the birefringence (Δn) of a liquid crystal as a function of applied electric field, demonstrating the optical anisotropy induced by molecular reorientation in a in an external electric field.

3.1.6. Fredericks Geometry

Molecules exhibit re-entrant behaviour at great electric fields are suitable for switching devices. The π-electrons donated by the biphenyl group and the electron of the Fluorine atom contribute to the enhancement of extraordinary rays for optical applications. The phenyl ring and connected cyclohexane ring decrease the π-electrons that are responsible for the decrement in optical anisotropy. The positive birefringence (Δn) was found to be 0.1446 for I52 liquid crystal. Birefringence is almost zero at low electric fields (0.00–0.02 a.u.), rising sharply to peaks around 0.14–0.16 beyond 0.04 a.u., due to transition. Two birefringence values, maximum value Δn_{max} = 0.1446 and another Δn = 0.146, indicating saturation of extraordinary-minus-ordinary refractive index difference. Figure 6 completes a trio of electro-optical responses, where birefringence emerges post-threshold (matching director angle onset in prior figure), peaking as refractive index stabilizes around 1.577–1.58. The linear rise and plateau align with nematic liquid crystal theory, quantifying Δn for applications like tunable waveplates or displays. Y-axis ranges from 0 to 0.16, capturing the full dynamic range of field-induced anisotropy.

3.1.7. Order Parameter

The order parameter (S) versus electric field of I52 liquid crystal is demonstrated in Figure 7. Liquid crystals can exhibit different types of order, including orientational order, positional order, and bond order. For the most common biaxial nematic liquid crystal, a second-rank symmetric traceless tensor order parameter is utilised to explain the orientational order of liquid crystals. The nematic phase is the least ordered and most basic liquid crystal phase; its order parameter is sometimes referred to as the scalar order or the order parameter modulus. There are multiple sharp peaks, each corresponding to a sudden increase in the order parameter, followed by a rapid decrease. S_{max} = 0.6863 appears in the upper right corner, indicating the maximum value of the order parameter observed on the graph. The periodic behaviour, with alternating peaks and valleys, suggests that this system is undergoing a periodic or oscillatory process, potentially related to the interaction between the electric field and the order parameter in the system being studied.

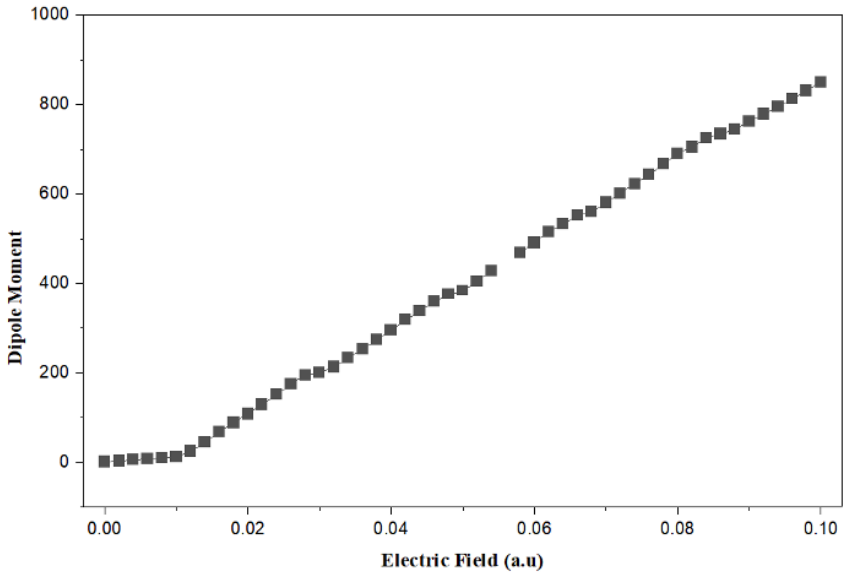

Fig. 2. Dipole moment v/s Electric field.

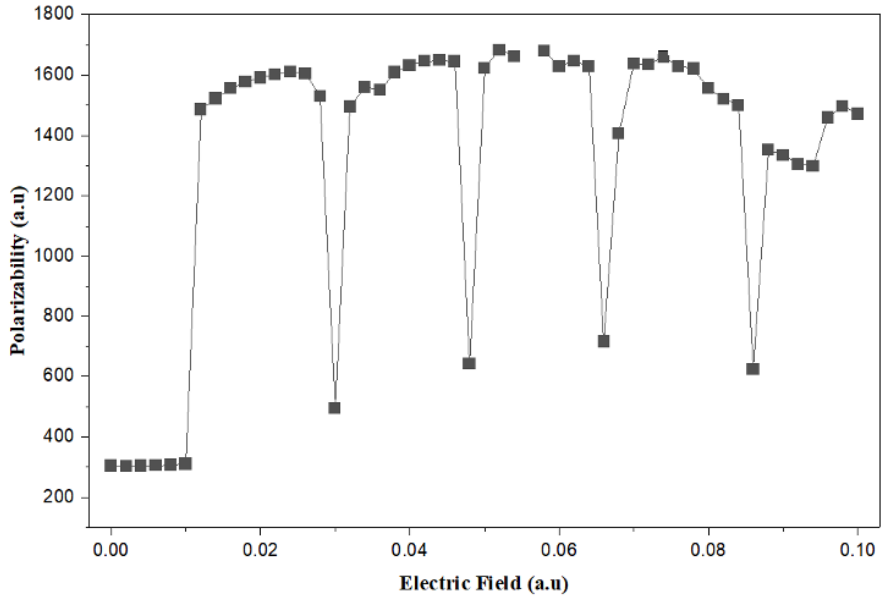

Fig. 3. Polarization v/s Electric field.

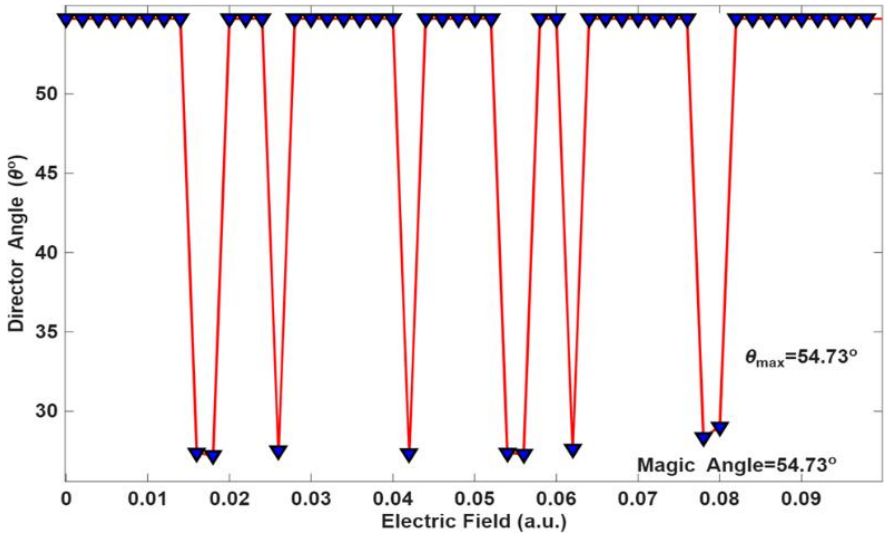

Fig. 4. Director Angle v/s Electric field.

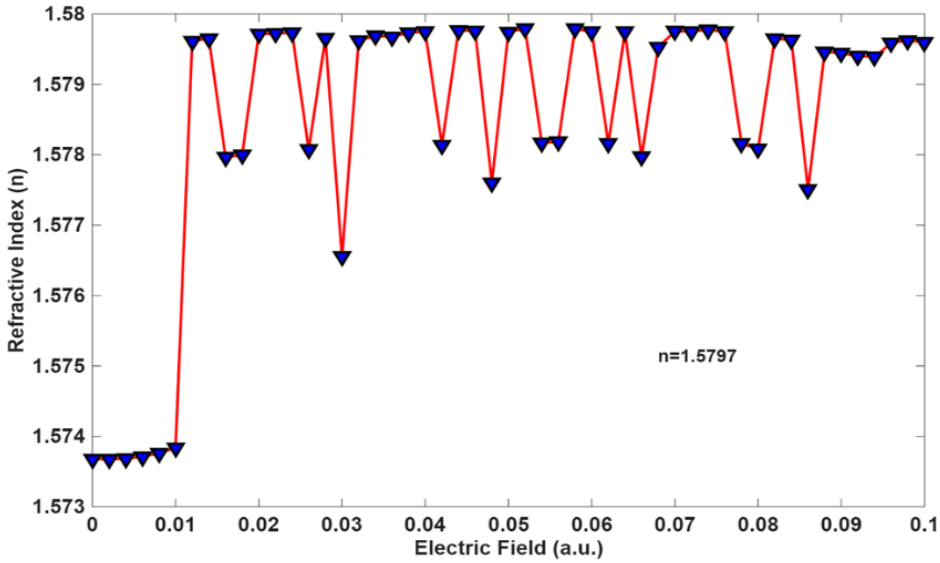

Fig. 5. Refractive Index v/s Electric field.

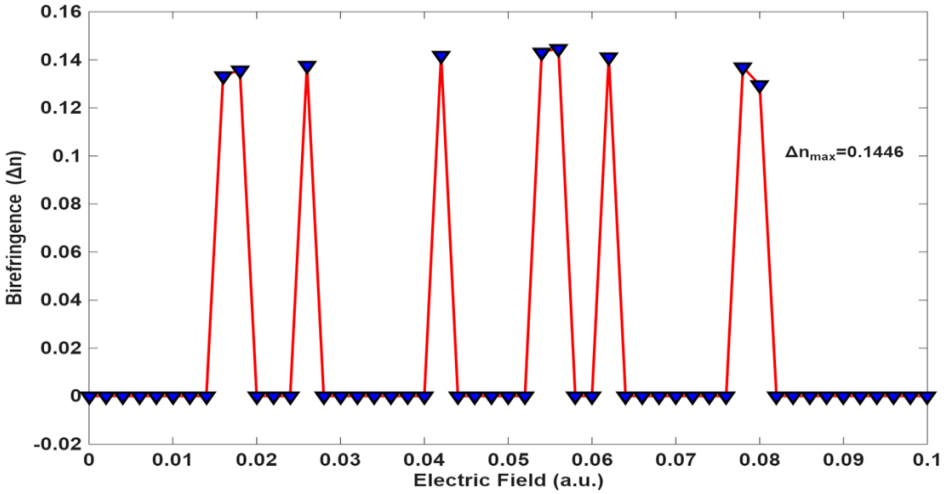

Fig. 6. Birefringence v/s Electric field.

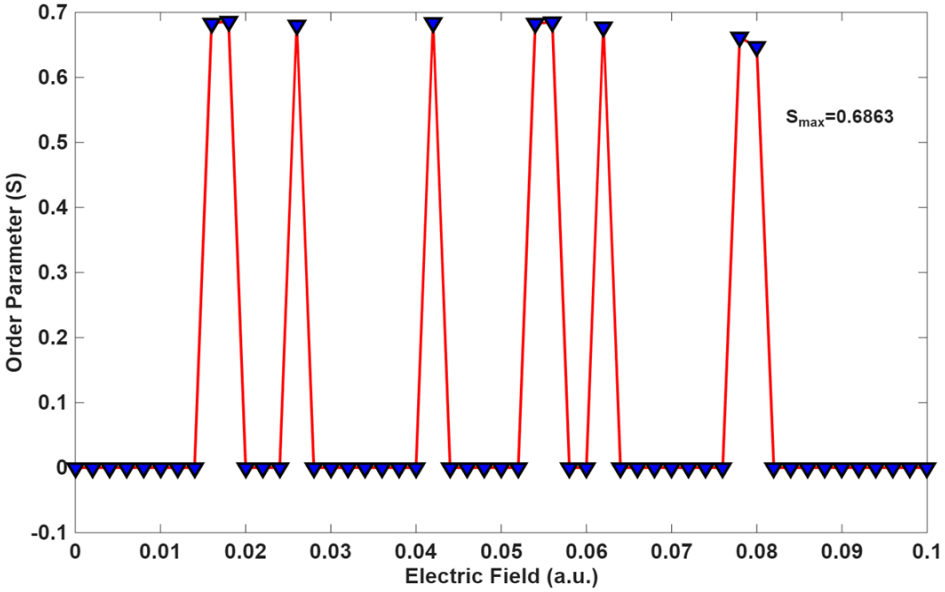

Fig. 7. Order Parameter v/s Electric field.

3.2. Electric-Field-Dependent Analysis of Thermodynamic Properties

Thermal energy (E in kcal/mol) versus external electric field is shown in Figure 8. At lower external electric field, I52 possesses 380 kcal/mole thermal energy. As the electric field varies from 0.00 to 0.10 a.u. the thermal energy decreases from about 380 kcal/mol to about 310 kcal/mol, showing that the more the field strength, the more the thermal energy gets less. While the overall trend is downwards, there are interesting fluctuations and minor peaks in the intermediate region (between 0.02 and 0.04 a.u.) due to structural or energetic transitions within the system with the increasing field. At lower external electric field, molecular arrangement of I52 remains unchanged due to strong intermolecular interactions. But as the external field increases these intermolecular interactions got weak and molecule possesses less thermal energy.

Fig. 9 displays the thermal correction of the enthalpy as a function of electric field. At lower external electric field from 0.00 a.u. to 0.01 a.u., enthalpy of the system remains almost unchanged. But as the electric field varies from 0.01 a.u. to 0.10 a.u., enthalpy of the I52 liquid crystal decreases. There are several prominent fluctuations including two deep local minima around the electric field values of 0.03 and 0.045 a.u. This is due to change in molecular arrangement at this particular electric field. This shows that enthalpy of the I52 liquid crystal is very sensitive to 0.03 a.u. and 0.045 au. electric fields.

Fig. 10 represents the variation of electronic energy + thermal free energy correction as a function of electric field along the x-axis. As the electric field goes from 0.00 to 0.10 a.u. the combined energy goes uniformly and smoothly from around -1151 Hartree to about -1168 Hartree, showing a nice and clean downward curve, but no abrupt fluctuation. This steady decline implies that the total energy for both electronic effects and thermal free energy corrections is increasingly stabilised (at a lower value) as the applied electric field increases. "EE + Thermal Energy Correction" in terms of the external electric field is represented by Figure 11. At lower electric field 0.00 a.u. to 0.01 a.u., "EE + Thermal Energy Correction" remains almost constant. As the value of the electric field goes from 0.01 to 0.10 a.u, the total energy (electronic energy plus thermal correction) of the system goes increasingly lower and the values reach around -1150 Hartree to approximately -1168 Hartree. This decrease in value with increasing electric field

is due to the change in molecular order indicating strong molecular order at lower values of the external electric field. The figure is particularly important to know field-induced changes in the energy of molecular or material systems, and to help realize that, even when energetics are considered in external fields, thermal corrections must be done.

Entropy is an important thermal property of the system which describes the degree of freedom or randomness of the system. Entropy of the I52 is very sensitive to the external electric field as shown in Figure 12. At lower values of the electric field particularly from 0.00 a.u. to 0.01 a.u., entropy of the system remains almost constant. But as the field varies from 0.01 a.u. to 0.10 a.u., entropy of the system decreases from 185 cal/mol-kelvin to 135 cal/mol-kelvin. The implication of this pattern is that, stronger electric fields decrease entropy of the system, possibly a sign of increase of the molecular order or decreased molecular freedom due to the influence of the field. Similarly, heat capacity of the I52 liquid crystal decreases with external electric field as shown in Figure 13. At lower values of the electric field particularly from 0.00 a.u. to 0.01 a.u., heat capacity of the system remains almost constant. But as the field varies from 0.01 a.u. to 0.10 a.u., heat capacity of the system decreases from 110 cal/mol-kelvin to 80 cal/mol-kelvin.

Fig. 14 shows the variation of "EE + Thermal Enthalpy Correction as a function of the applied electric field. At lower electric fields 0.00 a.u. to 0.01 a.u., "EE + Thermal Enthalpy Correction" remains almost constant. As the value of the electric field increases from 0.01 to 0.10 a.u, the total energy (electronic energy plus thermal correction) of the system decreases sharply from around -1151 Hartree to approximately -1166 Hartree. This trend indicates a strong stabilization effect in strong electric fields presuming caused by polarization or reorientation of dipolar species in the system by the field. The fact that we are including the thermal enthalpy corrections gives a thermodynamically relevant point of view, that both the enthalpic and electric contributions to the total energy are important.

Fig. 15 shows the dependence of zero-point energy on the external electric field. The zero-point energy decreases due to an increase in the strength of the electric field. There are a number of swings observable, among which is distinct sharp ridges and decadences, particularly where the values of electric fields go about 0.025, 0.035, and 0.10. a.u., indicating non-monotonic behaviour or may have instabilities in this range. Overall, the graph shows that the systematically lowering the zero point is achieved by the application of an external electric field.

Similarly, electronic energy (EE) plus zero-point as well as energy electronic energy (EE) decreases with external electric field as shown in Figures 16 and 17 respectively. As the value of the electric field goes from 0.01 to 0.10 a.u, the total energy (electronic energy plus thermal correction) of the system goes increasingly lower. This is due to strong molecular order in the system at high values of electric field, indicating the sensitiveness towards the external electric field. The trend corresponds to increase with stronger electric fields in the stability of the system, which reflects positions of the field-induced polarization and energy, and represents that polarization by the electric field takes place. The inclusion of zero-point energy does account for the quantum vibrational energy existing even at absolute zero temperature providing a fuller picture of the energetics of the molecular system in response to external fields. Such data are important in order to understand the molecular behaviour, energy landscapes, and potential phase transitions driven by electric fields in complex systems.

Figs. 18 and 19 represents Highest Occupied Molecular Orbital (HOMO) energy and Lowest Unoccupied Molecular Orbital (LUMO) energy as a function of Electric Field respectively. At lower electric fields 0.00 a.u. to 0.01 a.u., HOMO and LUMO energies remains almost constant. As the value of the electric field goes from 0.01 to 0.10 a.u, HOMO and LUMO energies decreases. This is due to polarization in the system. However, the energy band gap decreases from 5.08 eV to 0.2 eV at lower electric fields, i.e., from 0.00 a.u. to 0.01 a.u. But energy band gap remains almost constant (0.2 eV) in the range from 0.01 to 0.10 a.u, as shown in the Figure 20.

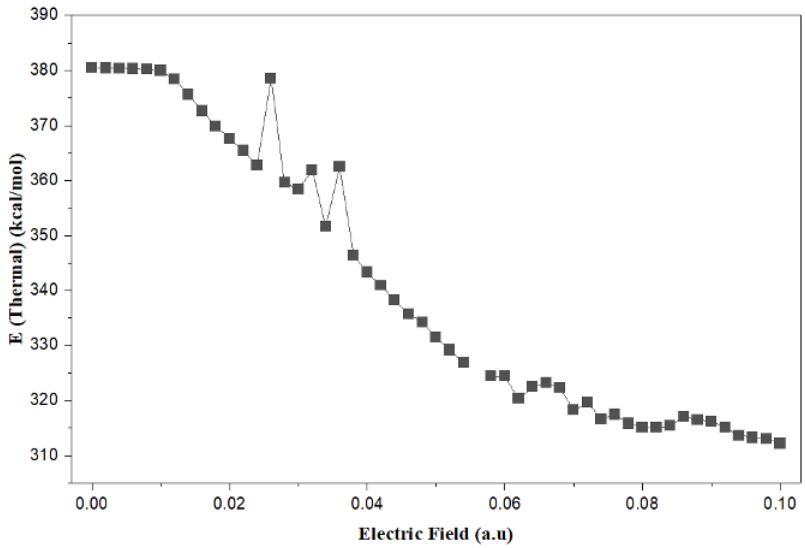

Fig. 8. Thermal energy v/s Electric field.

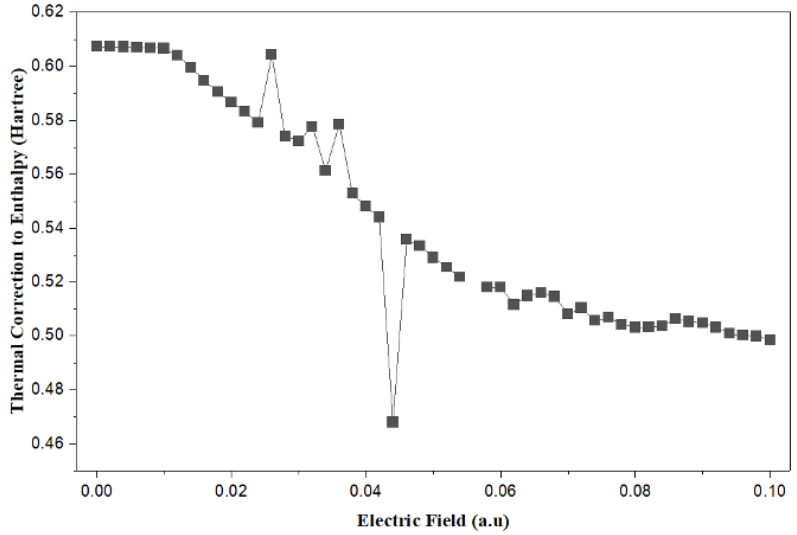

Fig. 9. Thermal correction to enthalpy v/s Electric field.

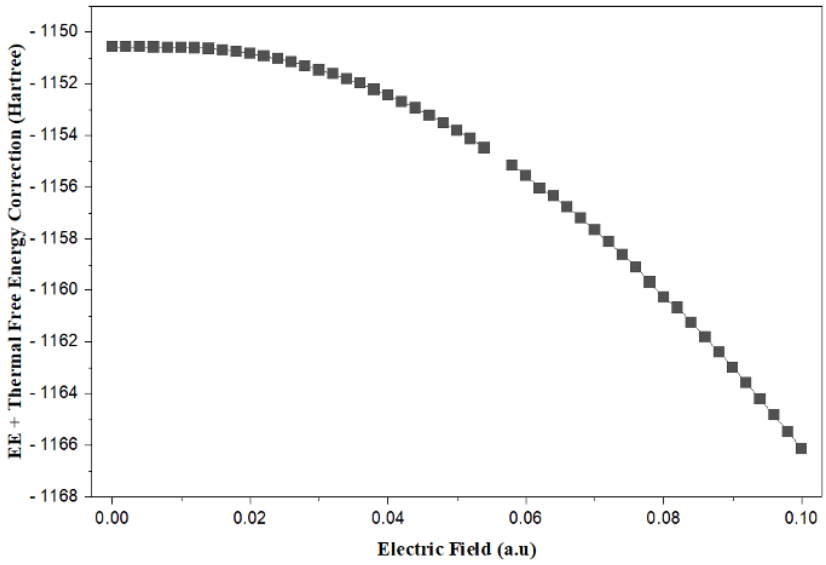

Fig. 10. EE+Thermal free energy correction v/s Electric field.

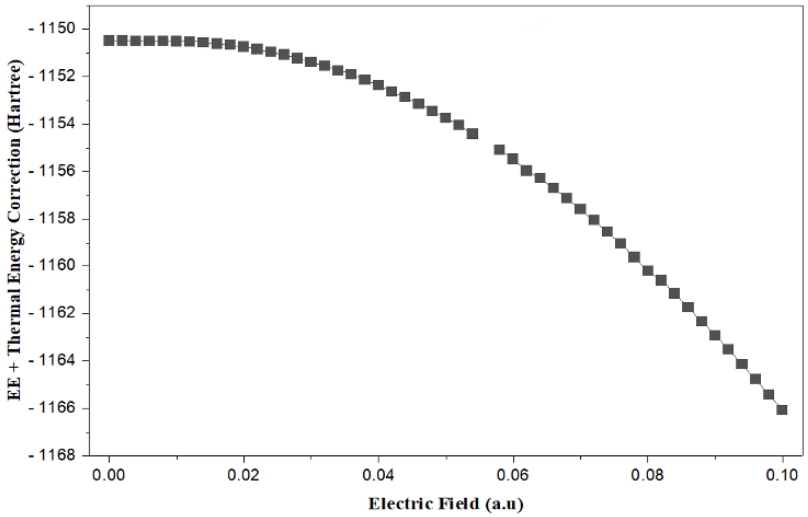

Fig. 11. EE+Thermal energy correction v/s Electric field.

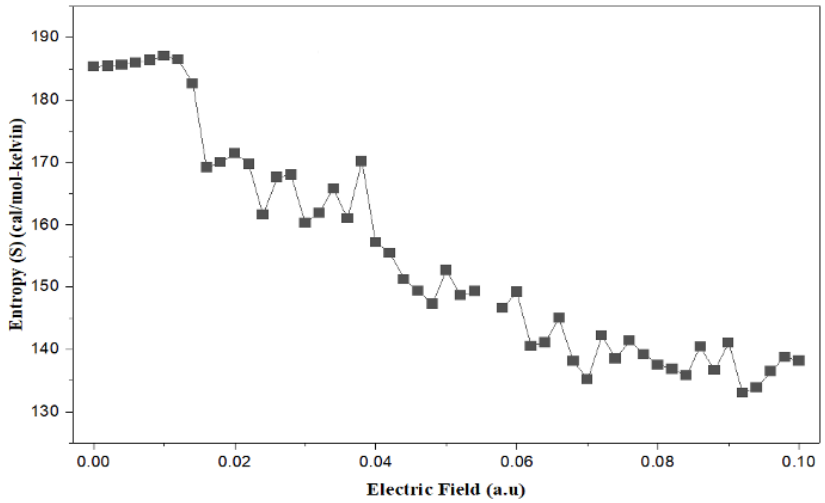

Fig. 12. Entropy(S) v/s Electric field.

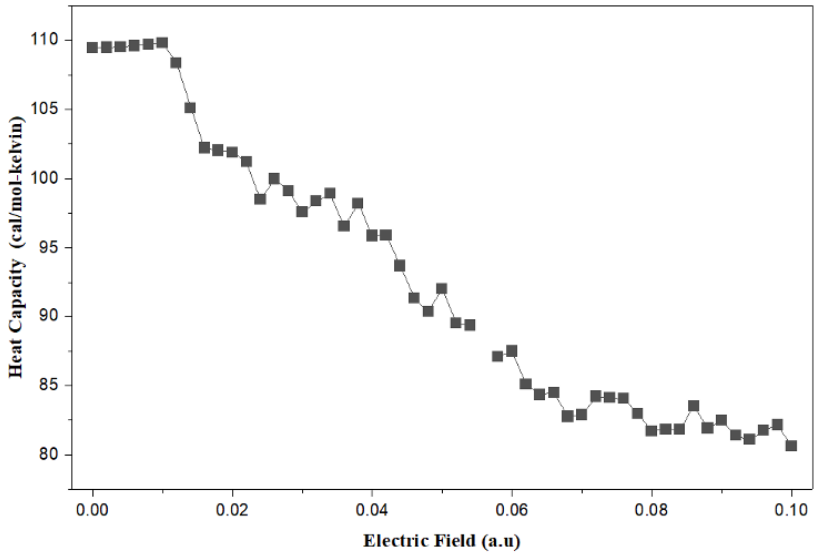

Fig. 13. Heat Capacity v/s Electric Field.

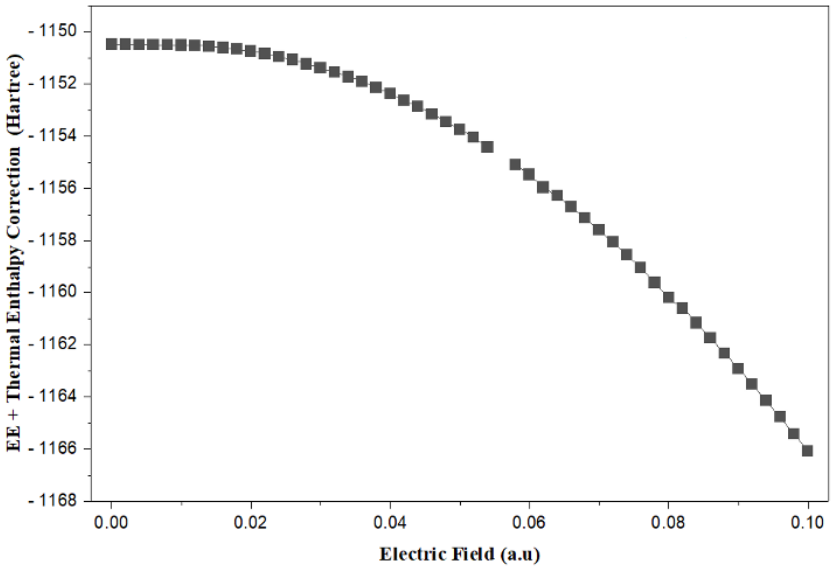

Fig. 14. EE+Thermal Enthalpy Correction v/s Electric field.

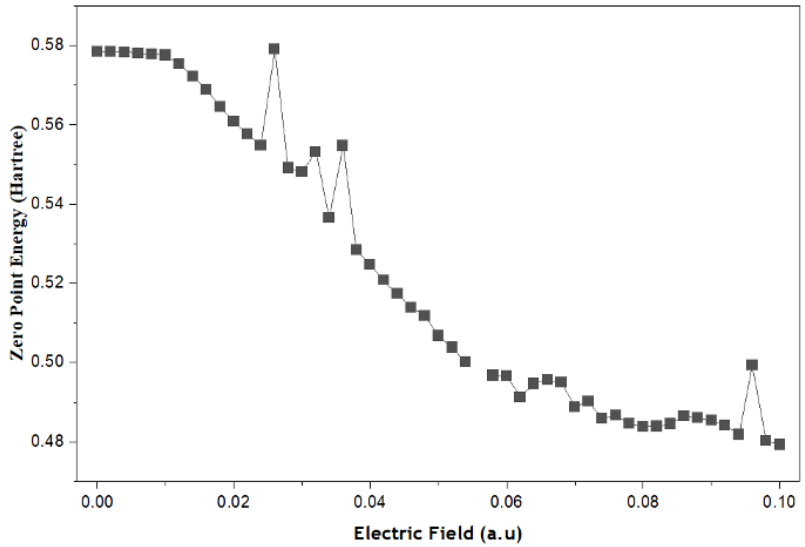

Fig. 15. Zero Point Energy v/s Electric Field.

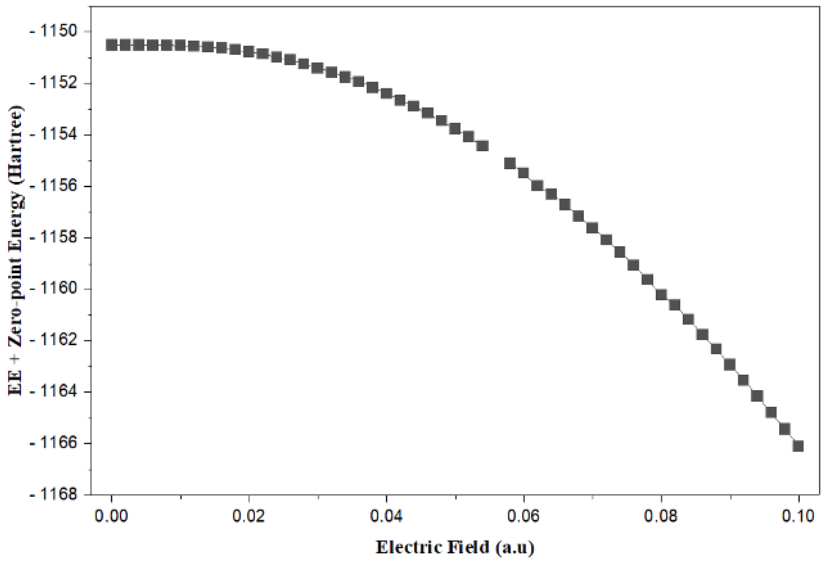

Fig. 16. EE + Zero-point Energy v/s Electric field.

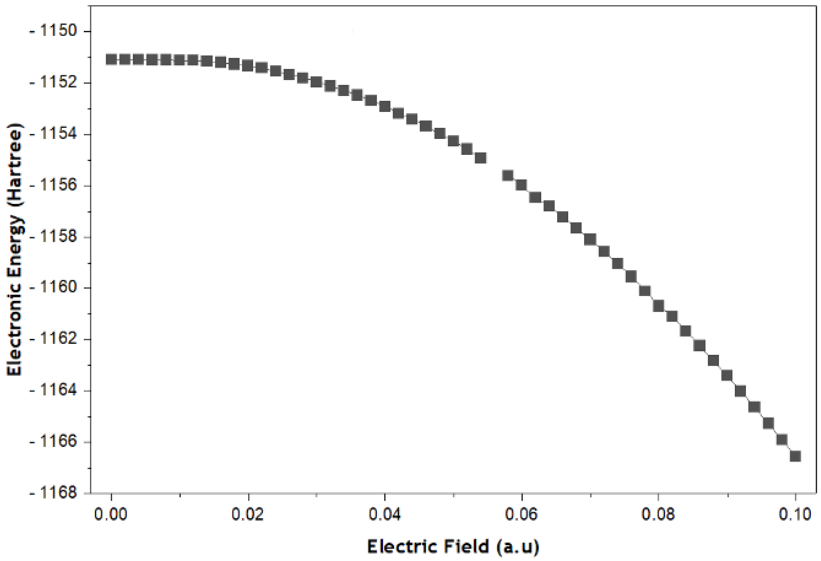

Fig. 17. Electronic energy v/s Electric field.

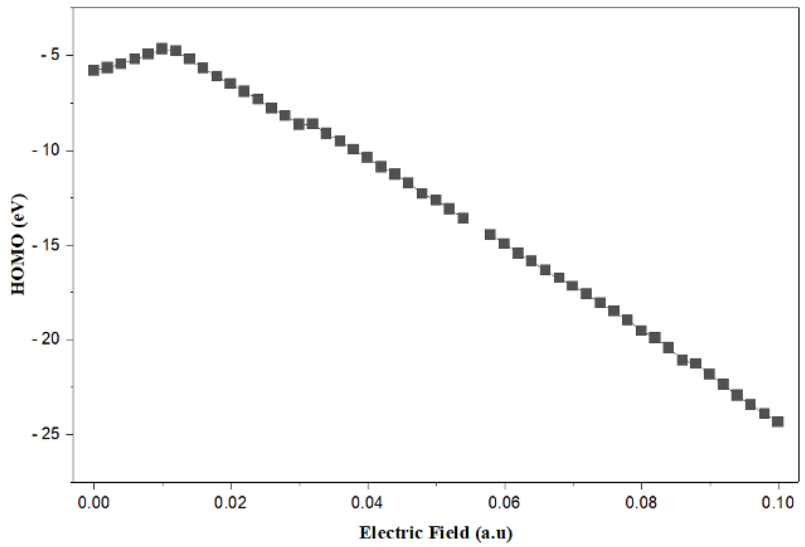

Fig. 18. HOMO v/s Electric field.

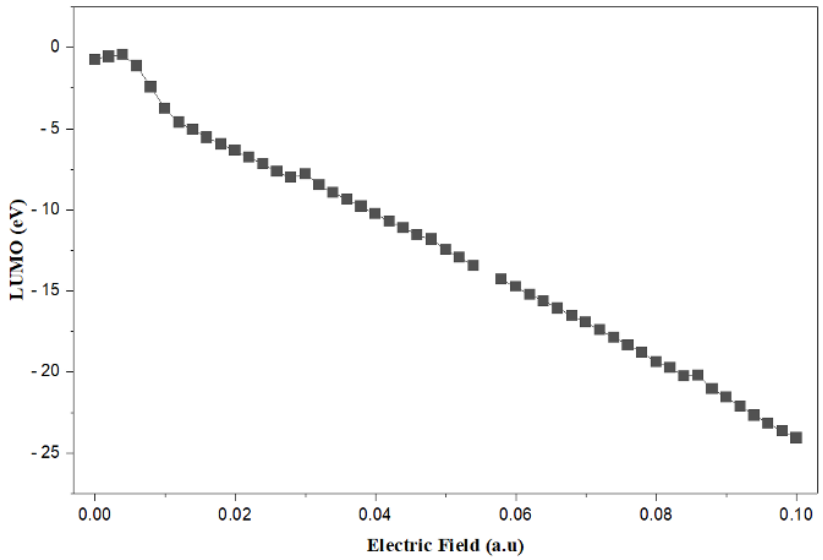

Fig. 19. LUMO v/s Electric field.

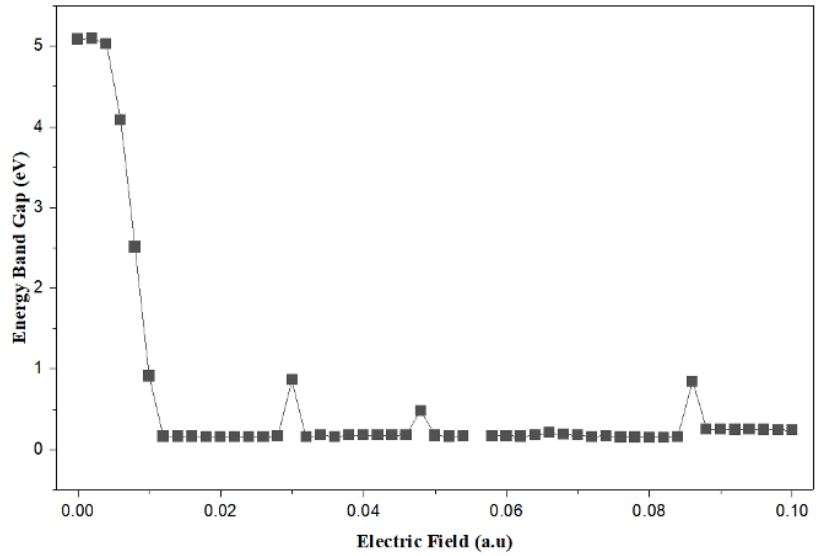

Fig. 20. Energy Band Gap v/s Electric field.

3.3. Spectroscopic Properties Analysis

3.3.1. FTIR analysis

FTIR analysis I52 liquid crystal is of great importance for the confirmation of chemical identity, analytical purity, and the functional group content of the advanced liquid crystal material [32, 34]. In canine absorption spectrum, FTIR spectrum of I52 presented in Figure 21 shows that there is clear absorption peaks associated to the aromatic and alkyl functionalities, which are typical of its biphenyl and cyclohexyl structures. The peak in the region 3000-2850 cm^{-1} is assigned to asymmetric and symmetric C-H stretching vibrations of the large number of alkyl side chains and trans-configuration of the pentylcyclohexyl moiety. The strong absorptions around the 1600 and 1500cm^{-1} are covered in the aromatic C=C stretching, indicates the rigid biphenyl core essential to be mesogenic. The other substituents, ethyl and pentyl, also have intense C-H bending vibrations in the region 1450-1370 cm^{-1} while the cyclohexyl rings produce minimal peaks associated with deformations in the chair conformers. It was clearly identified that the fluoro substituent is confirmed through a characteristic absorption in the range of 1000-1300 cm^{-1} which indicates the C-F stretching vibration that is not only confirmed by the presence of substitution but also influences dipole moment and molecular polarizability for electro-optic applications.

3.3.2. Raman Analysis

Raman spectroscopic study of I52 liquid crystal yields essential information concerning the molecular structure and dynamics of such complex liquid crystalline material. I52 molecular vibrational modes when irradiated with a particle-free (monochromatic) laser cause characteristic irradiation scattering (Raman effect), which appears as distinctive clusters of Raman spectrum [34]. Every peak shown in Figure 22, is associated with bonds and functional groups that are present: the biphenyl core usually has a strong correlation of the aromatic C-C signal of bonding in 1580-1600cm^{-1}, and the substituted ethyl and pentyl-cyclohexyl groups hinder additional links to be resonant as the groups characterized by C-H bonding (2800-3000cm^{-1}) and deformation of the rings. Fluoro substituent also affects the vibrational coupling, as C–F signals occur in the range of 1000 to 1100cm^{-1}, which give the spectral finger imprint of the halogenated surrounding.

3.3.3. UV analysis

Photophysical spectroscopy of I52 liquid crystal demonstrated by Figure 23, shows excitation bands that are important factors in understanding the photophysical behaviour and verifying the structural assignment of the excellent liquid crystal [33]. The molecular structure of I52 has an extended biphenyl core with ethyl and fluoro substituents appended onto it coupled with a trans-4-pentylcyclohexyl-ethyl to facilitate more conjugation and altered electronic distribution within the aromatic system. The characteristic UV absorbance profile with extensive p-p transitions characteristic for biphenyl derivatives with the maximum absorbance (l_{mx}) located in the range of 250-280 nm, which depends upon solvent and molecular orientation is observed in the figure.

The energy level spacing between HOMO and LUMO is modulated by electron-donating (ethyl), and electron-withdrawing (fluoro) substituents, which resulted in an effect on the peak position and intensity in the spectrum, in addition to the UV-vis absorption spectra. The UV spectrum of I52 is normally characterized by a narrow strong absorption band due to the biphenyl chromophore with optional weak hypochromic or bathochromic shifts due to solute-solute interactions and alkyl chain effects. The resulting trans-4-pentylcyclohexyl substituent, however, introduces rigidity to the molecule and consequently anisotropy, which affects to a small extent the absorption edge and causes slight spectral broadening relative to unsubstituted biphenyls.

The practical significance of the UV properties of I52 is an aspect of performances at liquid crystal devices, during which the electronic transitions of the material affect not only the light absorption but also the alignment of the molecules in an external field. Overall, these results of physio-chemical and optical properties demonstrate the potential of UV analysis as a useful tool in applied materials science to determine the molecular ordering, conjugation, and atomic precise effect on optical properties of I52.

3.4. Molecular Orbital Energy (MOE) Analysis

MOE analysis of I52 liquid crystal provides a rich understanding of molecular orbitals and optical properties of this complicated liquid-crystal molecule. The MOE spectrum shown in Figure 24 reveals population and strength of electronic states in energy levels providing the basis for understanding contributions from molecular orbitals and atomic fragments [35]. In I52, the p orbital structure of the biphenyl core plays a considerable role in the formation of the p-orbitals system, resulting in two clear peaks in the HOMO region, which corresponds to its conjugated aromatic system. Thanks to the presence of the fluorine atom at the 2-position, there are electronegativity and intense inductive effects, which modify the energy levels causing a downward shift of LUMO with a slight change to the HOMO-LUMO gap. The peaks of the MOE of the alkyl and cyclohexyl moieties are not so high but relevant to the elucidation of steric effects and the localization of the electron density which influences the stability of the phase and the formation of transition temperatures. Significantly, the MOE shows a moderate band gap, characteristics for the nematic liquid crystals, typical for the material's electro-optical applications. The broadening of the states in the vicinity of the frontier orbitals reflects the occurrence of hybridization of the biphenyl orbitals with the orbitals of the fluorine and alkyl substituents upon which the electronic coupling between the two hybridization results in changes in the way charge transport and polarization proceed. Generally speaking, the MOE of I52 demonstrates the sensitiveness of conjugation, electronegativity, and steric bulk content to tune the electronic character of the liquid crystal molecules, which, in turn, have been central to their selective functional activities associated with display and photonic devices.

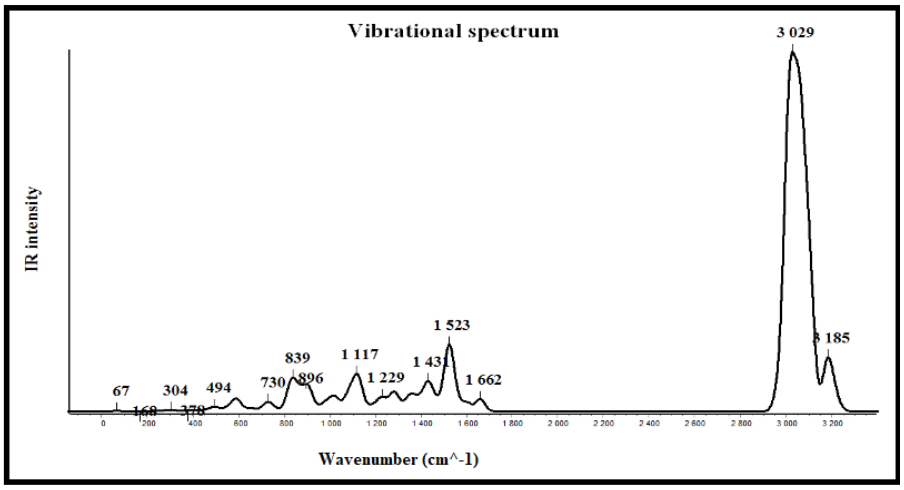

Fig. 21. FTIR spectrum of I52 liquid crystal.

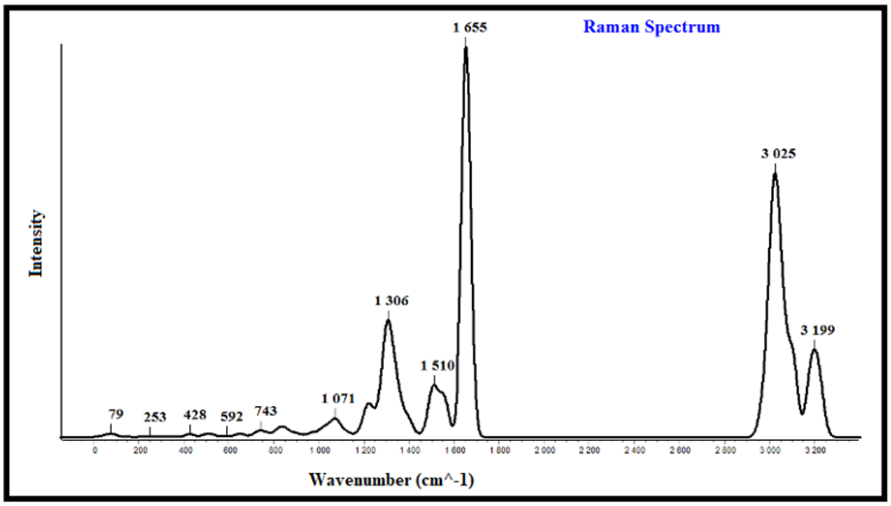

Fig. 22. Raman spectrum of I52 liquid crystal.

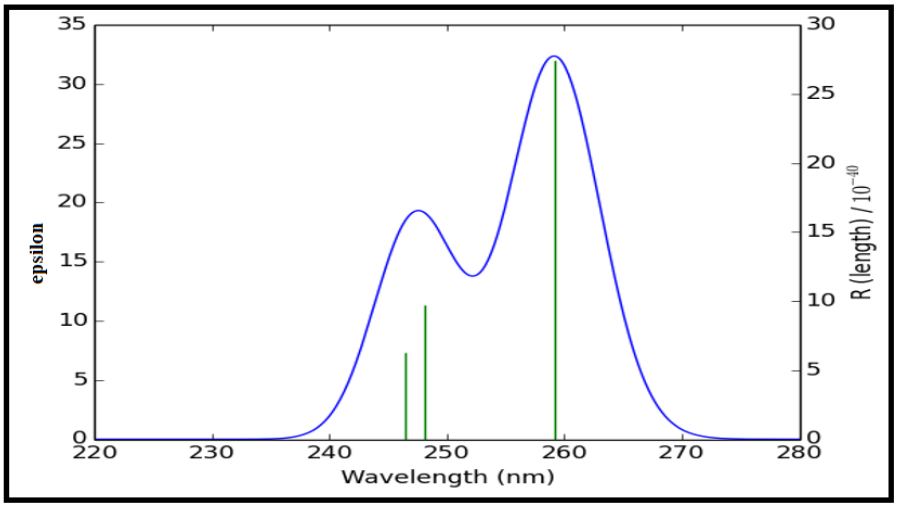

Fig. 23. UV spectrum of I52 liquid crystal.

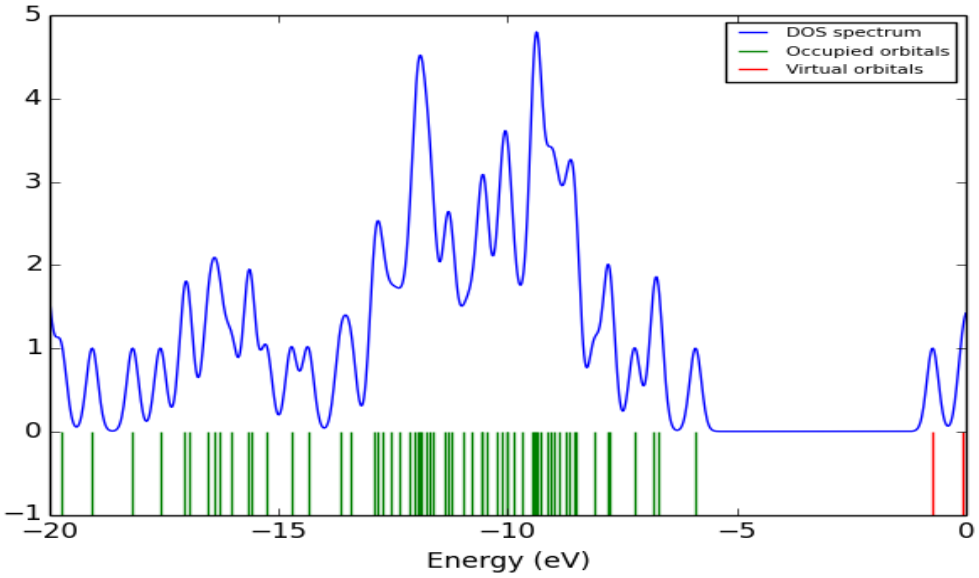

Fig. 24. Molecular Orbital Energy of I52.

4. Conclusions

In summary, the study of I52 liquid crystal shows that electronic properties such as dipole moment and polarizability of I52 increases linearly with external electric field due to field-induced effect. Opto-electronic property, i.e. birefringent shows that I52 is sensitive to external electric field and suitable for opto-electronic applications. Whereas the thermodynamical properties such as electronic energy (EE), thermal energy, enthalpy, entropy, heat capacity of the I52 decreases with external electric field. Thermal energy and enthalpy decrease with external electric field. This is because the system tends to have more molecular order as the external field increases. Zero-point energy graph shows that there is vibrational energy which exists at lower electric fields and decreases with increasing electric field. HOMO and LUMO decrease with external electric field. Energy band gap decreases first with external electric field and then becomes constant indicating that band gap is stable with external electric field. UV spectrum of I52 shows a sharp peak at 258 nm. Which indicates that I52 liquid crystal is sensitive to UV region. Raman spectrum confirms the presence of ethyl and pentyl-cyclohexyl groups due to C-H bonding in the range of 2800-3000cm^{-1}. FTIR spectrum confirms the C-H stretching vibrations at 3028 cm^{-1} due to alkyl side chains and trans-configuration of the pentyl-cyclohexyl moiety. Molecular orbital energy graph shows that the highest occupied molecular orbitals (HOMO) have high population density around -9 eV and -12 eV. HOMO-LUMO band gap is found to be 5.08 eV, which makes I52 suitable for insulating applications also.

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Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Authors Contribution Statement

Tikaram: Writing – review & editing, Writing – original draft. **Ravinder Kumar:** Writing – review & editing, Resources, Formal analysis. **Yogesh Kumar:** Computational Methodology, Data curation, Investigation, Validation, Conceptualization, Formal analysis. **Narinder Kumar**: Computational Methodology, Data curation, Investigation, Validation, Conceptualization, Formal analysis

Data Availability Statement

The data will be made available on a reasonable request.

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