

Phase Behaviour Estimation and Absorption Spectral Characteristics of Fluoro Liquid Crystals: Theoretical Approach

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Abstract

We adopted a theoretical approach to determine the preferred molecular pair configuration of 4'- (3,4,5-trifluorophenyl)-4-alkylbicyclohexyl (3FPnBCH) with n=3 (3FP3BCH), and n=5 (3FP5BCH) under translational and orientational motions. Detailed methodology has been described to calculate the interaction energies between a molecular pair. The configurational probability at transition temperature has been estimated using Maxwell-Boltzmann formula using interaction energy values as an input. Phase behaviour of the molecules has been analyzed using translational rigidity studies. Calculated UV absorption spectra using CNDO/S, INDO/S methods have been analyzed. The $\pi \rightarrow \pi^$ transitions, electro chemical properties based on HOMO, LUMO energies, and principal polarizability components, and anisotropy of polarizability have been reported to realize the kinetic stability, global reactivity, and non-linear optical activity of these molecules.*

Keywords: - *Probability; Polarizability; Anisotropy; optical activity*

INTRODUCTION

Liquid crystals (LCs) revitalization fundamentally, scientifically and technologically enables them as an omnipresent feature of everyday life. The research in fluorinated LCs (FLCs) has

been tremendously growing [1-2] as they enhance the range of all types of properties. New FLCs with wide phase exhibition have been frequently designed/synthesized, with interesting physico-chemical properties. The LC mixtures used

in high-resolution LC displays (LCD) contain highly fluorinated components, as, they shape the physical property profile of LCs [3]. It renders the materials healthier technically, thus enhancing the LCD manufacture and for cost reduction. The development of new FLCs is an important step to the realization of the true potential of LCs. However, many aspects of FLCs have been somewhat limited, and still truly remains a noteworthy task to researchers due to many challenges [4-5].

The uncontrolled mobilization of ions is the key problem with many polar substituents, which leads to decrease of voltage holding ratio, contrast diminution, or image sticking. Fluorine/ fluorine-containing functional groups are amazing alternative for this problem to prevail the said issues. Since, fluorine is the most electronegative element; it offers strongly polarized bonds with other electro-positive elements such as carbon to generate substantial dipole moment. Therefore, terminal group with fluorine offers the LC with a positive dielectric anisotropy, and dipole moment along the molecular axis. The complexities linked with highly conjugated LCs are large melting points, enhanced viscosity, low resistivity, and lower UV stability [6]. Among these, the UV stability is considered to be the tricky

aspect with respect to different types of substituents and solvents [7-8]. However, knowledge on the factors responsible for mesophase formation is essential to establish molecular models. Further, the opportunity also exists of out spreading these models by establishing the accurate features such as molecular rigidity [9], anisotropy [10], asymmetry [11], and electrostatic forces [12]. The anisotropy of molecular interaction is usually approved as the prerequisite to model the thermotropic LC [13].

The intermolecular forces are highly important in estimating the various orders of mesogens. The sequence of liquid crystallinity and transition temperature is directed via the forces that work between the sides, planes and ends of a molecular pair. The detailed analysis of pair interactions between the molecules is probable to provide enough knowledge of mesomorphism. Hence, the estimation of various relative configurational probabilities has been carried out.

An effort has been made to estimate the phase behaviour of 3FPnBCH (n=3, 5) compounds using the configurational probabilities. The stacked structures have been arranged with 7Å distance, in-plane mode with 9Å, and 24Å has been fixed for

terminal mode. These distances have been maintained to nullify the van der Waals contacts. Moreover, these distances allow the short- and also intermediate-range interactions for a molecular pair. The literature data shows that the transition temperatures for 3FP3BCH are 366.7K [14], and 3FB5BCH is 375.4K [15].

Further, the semi empirical analysis is expected to offer an insight into molecular absorption, electro-chemical, and optical properties using the CNDO/S [16, 17], INDO/S [18, 19] schemes. Global chemical reactivity descriptors are reported to understand stability and reactivity, while polarizability components are analyzed to understand the nonlinear optical activity.

MATERIALS AND METHODOLOGY

The structures of 3FP n BCH ($n=3, 5$) have been generated using the reported data [14, 15]. A position that is nearer to the centre of mass of the structure has been selected as origin. Along the molecular long axis; X-axis has been fixed. The Y-axis has been taken in the plane of the structure, and Z-axis perpendicular to the plane of the molecule. The CNDO/S approach [20] has been implemented to estimate the atomic net charge and dipole moment. The

following methodologies have been implemented in three parts:

Interaction energy

By employing the modified second order perturbation theory for medium range interactions [21], the total interaction energy (E_{total}) for a molecular pair is given by

$$E_{\text{total}} = E_{\text{el}} + E_{\text{pol}} + E_{\text{disp}} + E_{\text{rep}}$$

where E_{el} is electrostatic, E_{pol} is polarization, E_{disp} is dispersion, and E_{rep} is repulsive energy components. Further, the electrostatic term is expanded as

$$E_{\text{el}} = E_{\text{QQ}} + E_{\text{QMI}} + E_{\text{MIMI}} + \dots$$

where E_{QQ} is monopole-monopole, E_{QMI} is monopole-dipole and E_{MIMI} is dipole-dipole terms respectively. The addition of higher order multipoles does not alter the electrostatic interaction energy significantly. Hence, the calculation has been done only up to dipole-dipole term [22]. The detailed methodology and formulae have been reported in the literature [22].

Configurational probability

From the above step, the estimated total interaction energy values have been used

as an input to calculate the probability of each configuration using the Maxwell-Boltzmann formula [23]:

$$P_i = \exp(-\beta \varepsilon_i) / \sum_i \exp(-\beta \varepsilon_i)$$

where P_i represents the configuration probability, ε_i is the energy of configuration i relative to the minimum energy configuration. k represents the Boltzmann Constant, and T is the absolute temperature.

UV-Vis absorption spectra calculation

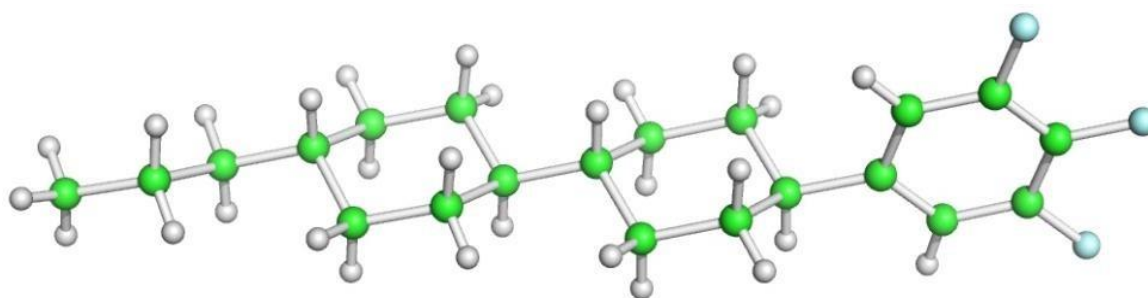
The absorption spectra have been calculated using CNDO/S, INDO/S approximations, which are the forms of the CNDO, and INDO methods reparametrized to replicate the excitation energies obtained through experiment. The UV absorption data has been estimated via the CI method that is based on attained multi-electron wave functions. In this CIS method [24], the orbitals of the H-F solution have been utilized to produce singly excited determinants. This way of dealing may be understood as the H-F analysis for excited states [25]. The electron correlation has not been included

in the CIS method, which is an analog of the H-F procedure for the excited states.

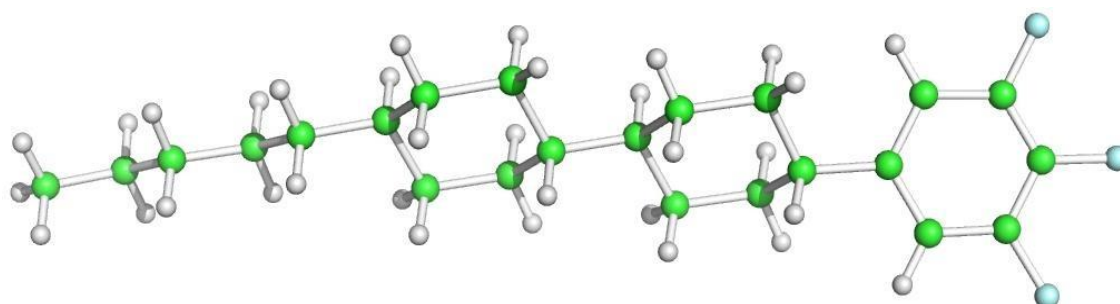
The ZINDO [26, 27] has been precisely parameterized to estimate the theoretical transition energies, and the corresponding intensities of organic molecules in the UV-Vis region with a certain CI expansion of singly excited determinants. The frontier molecular orbitals (FMOs) such as HOMO and LUMO, denotes the tendency to donate or accept the electrons respectively. This tendency plays vital part in its optical, electrical properties and in chemical reactions. The electro chemical properties of 3FPnBCH structures using CNDO/S, INDO/S methods have been described based on HOMO and LUMO energies. Further, the principal polarizability parameters have been calculated (Table 4) to understand the non-linear optical activity of these structures.

RESULTS AND DISCUSSION

The structures of 3FP3BCH and 3FP5BCH molecules have been reported in Fig. 1



(a) 3FP3BCH



(b) 3FP5BCH

Fig. 1 Molecular structure of (a) 3FP3BCH (b) 3FP5BCH

The configurational probability distribution corresponding to the various modes of interactions has been analyzed below:

Probability distribution during stacking mode

In a molecular pair, one molecule has been placed in x-y plane, whereas the second molecule has been shifted by 7 Å along z-axis with respect to the molecule fixed. The probability distribution during the rotational motion about Z-axis for the configuration x (0°) y (180°) has been estimated. It has been noticed that the probability maxima corresponding to

3FP n BCH ($n=3, 5$) molecules exhibits a prominent preference. Hence, the energy minima attained here is then considered as input. Further, the procedure has been continued for smaller rotations. This step reveals that optimum inter-planar distance for 3FP n BCH molecular pair depends on the rotations given about x- and y-axes. The configuration is further examined via very small intervals of distance and angle. A translational precision of 0.1 Å in and rotational precision of 1° for one molecule with respect to other has been attained.

The distribution of probability corresponding to the configuration $y(0^\circ)z(0^\circ)$ with respect to translation along the molecular long axis has been reported in Fig. 2. Evidently, the configurations show a definite inclination for the energy minimum point. The probability variation of is nearly identical for region $-1.2\text{\AA} \pm 0.4\text{\AA}$. This region is favorable for the molecules to slide one over the other. This phenomenon may be linked with the

fluidity of molecules preserving its ordering in mesophase.

Fig. 3 represents the distribution of probability with respect to rotation about x-axis for configuration $y(180^\circ)z(0^\circ)$. The maximum probability corresponding to 3FP3BCH and 3FP5BCH at -1° and $+1^\circ$ respectively shows a small preference for an associated structure for this configuration at phase transition temperature.

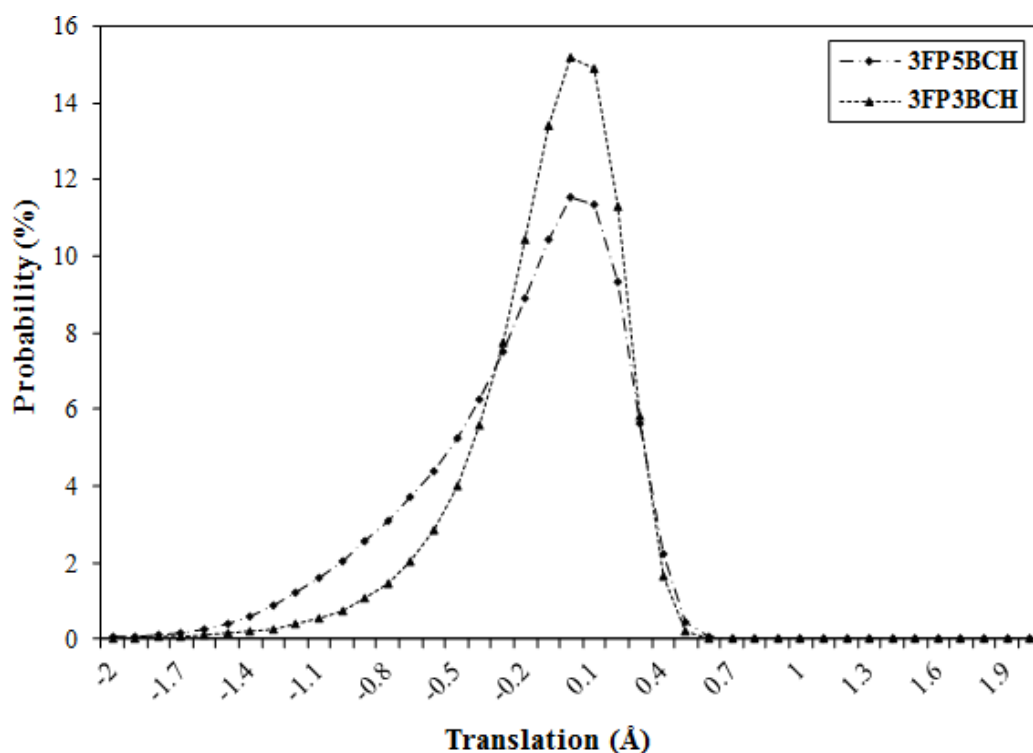


Fig. 2 Variation of probability with respect to translation along x-axis during stacking interactions for configuration $y(0^\circ)z(0^\circ)$ at N-I transition temperature

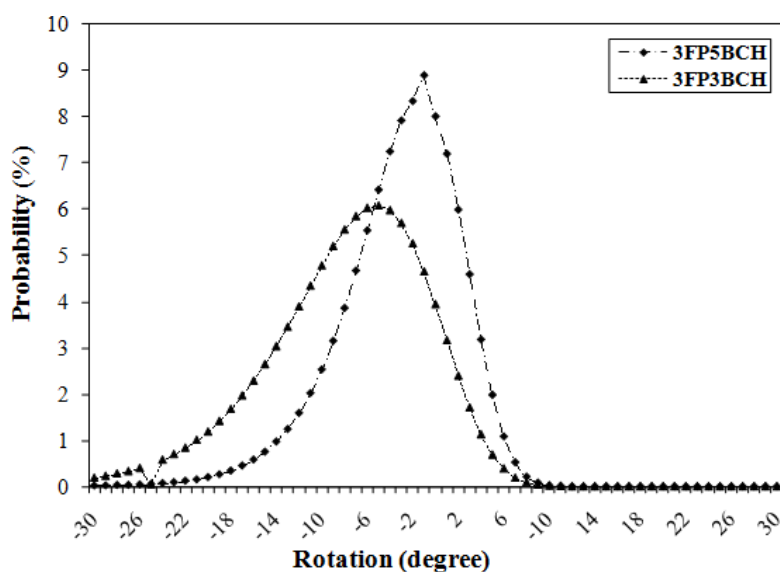


Fig. 3 Variation of probability with respect to rotation about x-axis during stacking interactions for configuration y (180°) z (0°) at N-I transition temperature

Probability distribution during in-plane mode

During in-plane mode, one of the interacting molecules has been arranged at a distance of 9Å along y-axis with regard to the fixed molecule. The effect of translation corresponding to the configuration y (00) along x-axis has been reported in Fig. 4.

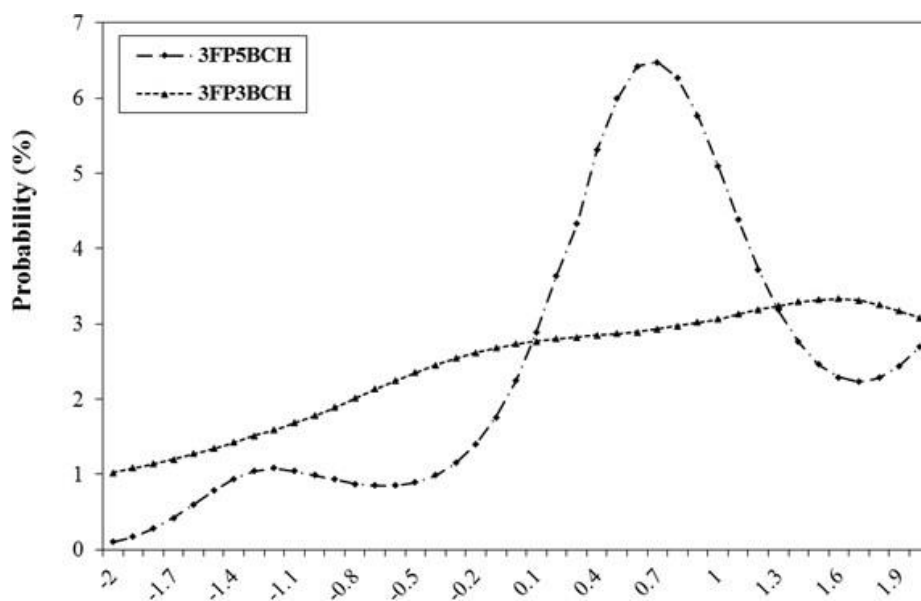


Fig. 4 Variation of probability with respect to translation along x-axis during in-plane interactions for configuration y (00) at N-I transition temperature

It has been understood that the molecular pair possesses a greater translational freedom. This is a consequence of weaker in-plane interactions to the stacking interactions. Further, the interacting configuration has been refined during translational operation along x- and rotational operation about y-axis at equilibrium state, the energy has been minimized. The calculated probability has been furthermore analyzed with respect to rotational motion about x-axis. The probability distribution with respect to rotational motion about x-axis corresponding to the configuration y (1800) has been examined. The significant maxima in probability have been observed near the equilibrium point.

Further, it may be noticed that the rotational flexibility is higher (*i.e.* small change in energy) compared to stacking interactions. Since, the in-plane electrostatic energy is more effective to the stacking component, and higher pole interactions become less effective even if taken into consideration, the variation in the configurational probability is expected to be altered. Larger translational freedom has been noticed as compared to stacking mode. Translational variation along y-axis has also been analyzed which reveals that

smaller translation along y-axis does not considerably vary the total energy.

Probability distribution during terminal mode

The terminal mode is in general very much weaker in comparison to stacking and/or in-plane mode of interactions. The effect of rotation about x-axis for configuration y (00) for molecule kept at 24Å separation in x-direction has been studied. It has been noticed that the molecules in this mode exhibits highest rotational freedom about their molecular long axis. Further, probability maxima have been noticed corresponding to various inclinations.

It is of significance to note here that the dispersion forces contribute largely in stabilizing interacting pair of 3FPnBCH (n=3, 5) molecules during all modes of interactions. This is also in agreement with the basic concepts of molecular field theory [22-24].

ESTIMATION OF PHASE BEHAVIOUR

To estimate the phase behaviour, the following rigidity analysis has been taken into focus.

Translational rigidity

Table 1 reports the translational rigidity parameters at various temperatures along the molecular long axis for 3FP3BCH, and 3FP5BCH during stacking and in-plane interactions.

Translational molecular rigidity has been estimated as the ratio of maximum probability at a particular translation point to having + 0.1Å displacement along the molecular long axis. It may be noticed that the rigidity parameter is 0.53 at transition temperature (366.7K) for 3FP3BCH, and the value is 0.55 at room temperature (300K) representing a higher ordering at low temperature. An increment in temperature causes the molecules to gain adequate flexibility to glide along the molecular long axis. This freedom with respect to translation has been found to be

is more dominant in planar interactions. Evidently, the parameter is found to be 0.51 at 300K that decreased to 0.48 at transition temperature (366.7K). It may be concluded from the above data that significant flexibility has been noticed for smaller translation. Further, longer intervals of translation are not generally allowed, as it may not offer the detailed picture in terms of freedom. Thus, in the region of mesomorphism, it is only possible to observe small movements of molecules. Hence, it may be accomplished that the molecule is quite freer for translation during in-plane mode of interactions. The relative analysis shows that the pair of molecules does not show any inclination to form stacked layers. This establishes the nematic phase behaviour of the molecules.

Table 1 Translational rigidity parameters along the long molecular axis (x-axis) as a function of temperature during stacking, and in-plane interactions of 3FP3BCH, and 3FP5BCH molecules.

Molecule	Temperature/ K	Stacking mode	In-Plane mode
3FP3BCH	300	0.55	0.51
	366.7*	0.53	0.48
3FP5BCH	300	0.55	0.51
	375.4*	0.54	0.49

UV-Vis absorption spectra, electro-chemical, and non-linear properties

The UV spectra of various molecules depend on the electronic transitions which involves π and/or n electron systems. The interaction of light with LC compounds is of higher attention to expand the possibility to design novel display appliances. The study of atomic charge, transfer of excitation energy that occurs in various absorption mechanisms of LCs needs quantum chemical approaches. These basic approaches verify the viability of such mechanisms in display and other photonic appliances. The molecular structure, excited states, and the electro-chemical, non-linear optical properties must be described for LC models for the complete picture of molecular orbitals [28]. This offers an account of the chronological process for improving the UV absorption, and response time of the designed molecules. The configuration interaction (CI) approach is extensively in use for the study of electronic spectra. The absorption analysis of larger molecules and LCs becomes possible by coupling CI method coupled with a model semi-empirical Hamiltonian [29]. The UV absorption analysis of 3FPnBCH ($n=3, 5$) structures have been given below based on CNDO/S, INDO/S methods.

4'-(3,4,5-trifluorophenyl)-4-propylbicyclohexyl (3FP3BCH)

The UV absorption data of 3FP3BCH molecule using CNDO/S, INDO/S approaches has been shown in Fig. 5 and 6 respectively. A two-band data has been noticed corresponding to UV wavelength with absorption bands at 216.40nm (λ_1), and 265.03nm (λ_2) based on CNDO/S method. No other absorption has been noticed corresponding to the visible wavelength. The INDO/S method estimates a strong absorption at 271.48nm only. These bands (CNDO/S: 265.03nm, INDO/S: 271.48nm) take places because of the HOMO $\rightarrow$ LUMO transition and designated as $\pi\rightarrow\pi^*$ transitions. Further, the remaining absorption bands at other UV wavelengths also specify the probability of additional $\pi\rightarrow\pi^*$ transitions.

4'-(3,4,5-trifluorophenyl)-4-pentylbicyclohexyl (3FP5BCH)

The UV absorption data of 3FP5BCH molecule using CNDO/S, and INDO/S approaches has been shown in Fig. 5 and 6 respectively. A single band has been identified corresponding to the UV wavelength with absorption bands at 263.28nm (CNDO/S), and 270.31nm (INDO/S). Further, no absorption band has been identified corresponding to the

visible wavelength. These absorption bands take place due to the HOMO→LUMO transition and designated

as $\pi \rightarrow \pi^*$ transitions. In this way an accord has been observed in calculating the absorption data (Table 2).

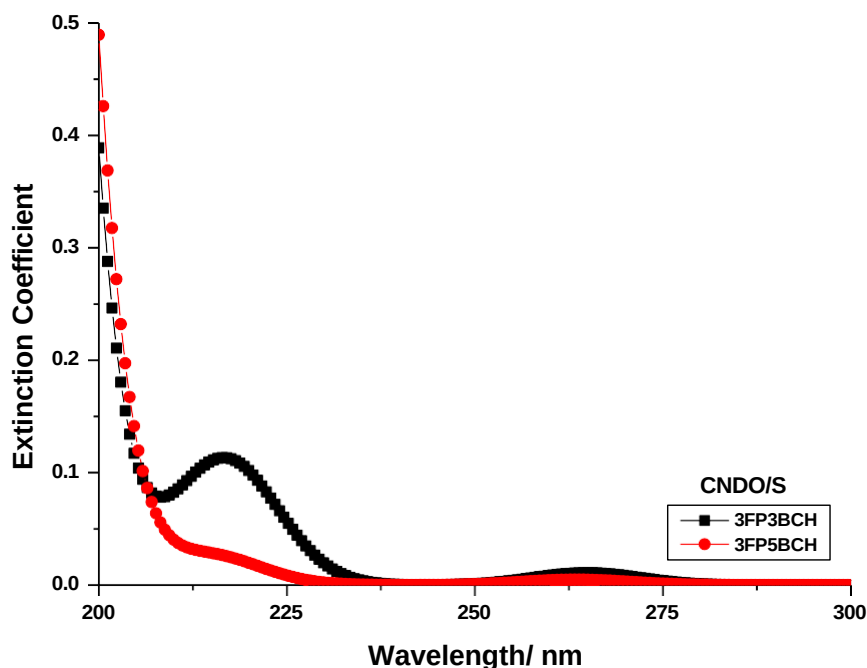


Fig. 5 UV absorption spectra of 3FPnBCH (n=3, 5) molecules using CNDO/S method

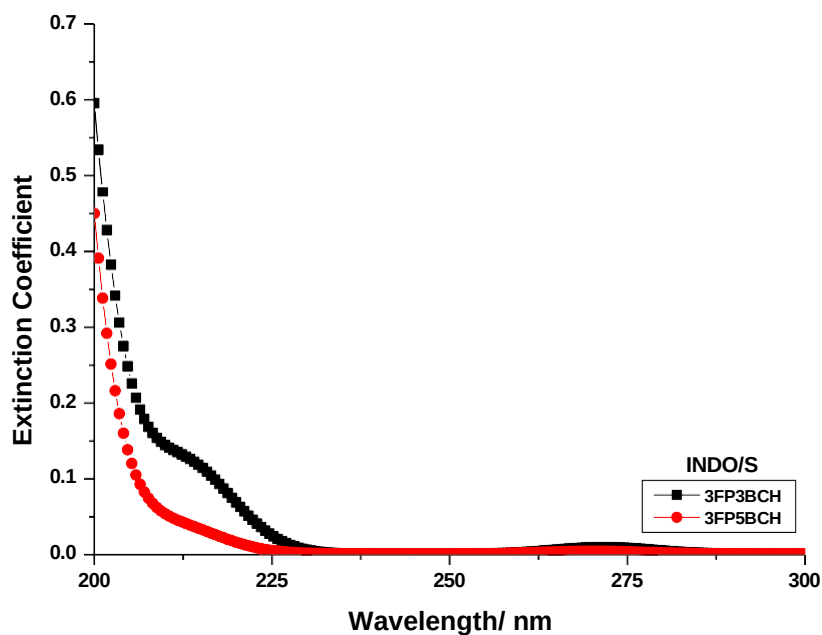


Fig. 6 UV absorption spectra of 3FPnBCH (n=3, 5) molecules using INDO/S method

Table 2. The absorption maxima (λ_{max}), extinction coefficients, oscillator strength (f), vertical excitation energies (E_v), dipole moment (μ) and its components (μ_x , μ_y , μ_z), HOMO (H), LUMO (L), and energy gap (E_g) of 3FP3BCH, and 3FP5BCH molecules using the CNDO/S, and INDO/S methods.

Molecule	Absorption bands/ nm	Extinction**	E_g / eV	f	μ_x	μ_y	μ_z	μ / D
3FP3BCH								
CNDO/S	216.40	0.11	5.72	0.11	1.38	0.76	-6.01	6.21
	265.03*	0.01	4.68	0.01	1.34	0.75	-5.42	5.63
	H= -9.86eV	L= -0.96eV	E_g = 8.90eV					
INDO/S	271.48*	0.009	4.56	0.009	1.34	0.63	-5.29	5.49
	H= -8.93eV	L= -0.11eV	E_g = 8.82eV					
3FP5BCH								
CNDO/S	263.28*	0.004	4.71	0.004	0.80	0.43	-5.59	5.66
	H= -10.19eV	L= -1.21eV	E_g = 8.98eV					
INDO/S	270.31*	0.003	4.59	0.003	0.79	0.46	-5.43	5.51
	H= -9.23eV	L= -0.34eV	E_g = 8.89eV					
* λ_{max} / nm		**Extinction unit: $10^4 \text{ dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$						

ROLE OF SUBSTITUENT IN SPECTRAL SHIFTS

The absorption spectra of 3FPnBCH compounds have been reported in Table 2. It may be noticed from the table that addition of two alkyl groups in 3FP3BCH has major part in the absorption band shift. The CNDO/S data reveals that 3FP3BCH has absorption maxima (λ_{max}) at 265.03nm, and 3FP5BCH at 263.28nm. Hence, the additional alkyl groups cause a blue shift and hypochromic effect. A detailed report of the wavelengths corresponding to absorption, extinction values (EC), oscillator strength (f), excited energies (E_v), in UV region,

dipole moment and its components, the energies of HOMO, LUMOs, and energy gap values using the CNDO/S, INDO/S approaches have been shown in Table 2. Similarly, INDO/S method also estimates a blue shift with hypochromic effect that is due to charge transfer within the molecule due to added alkyl groups.

The blue-shift (substituent induced) of absorption wavelength leads to an increase in excited energies through which spectral parameters are altered. An increment in the HOMO, LUMO (magnitude wise) and energy gap values has been noticed due to the addition. Further, considerable

agreement has been observed in estimating the absorption maxima. Due to the excited electron, the absorption peak will result into poor interaction electrostatically. This causes a blue shift, and point chromophores towards a dominant exciton coupling. Since, 3FP5BCH has relatively stable phase, the increase in the transition energies has been expected. This leads the absorption band towards weaker electrostatic interaction. Further, due to this the effected charge distribution causes a decreased delocalization of electrons. Hence, no $n \rightarrow \pi^*$ transition occurs at ground, and excited levels. This confirms the lesser values of rigidity (Table 1) of the molecules. The assessment of absorption peaks reveals that 3FP3BCH has higher photo sensitivity, lower band gap, and high conductivity.

DIPOLE MOMENT, FRONTIER MOLECULAR ORBITALS AND ELECTRO CHEMICAL PROPERTIES

The dipole moment is an electronic property that arises due to the non-uniform charge distribution of atoms in the molecule. From Table 2, it may be observed that the dipole moment values increase from 3FP3BCH to 3FP5BCH. This variation of dipole moment (and

polarizabilities also) may require an insight into the molecular HOMOs and LUMOs generated. The HOMOs and the LUMOs are designated as frontier molecular orbitals (FMOs). The HOMO (H) signifies the electron donating ability; LUMO (L) signifies the ability to attain an electron. These play an important role in its electro-chemical, absorption, and non-linear optical properties and in several reactions. The gap between H, L energies estimates the kinetic stability, optical polarizability, chemical reactivity, and hardness-softness of a molecular structure.

Table 2 indicates that the H, L, and energy gap values of 3FPnBCH molecules using CNDO/S, INDO/S approaches. The chemical hardness, reactivity, potential, softness, electro negativity, kinetic stability, electrophilicity, and optical polarizability, etc. of a molecular system can be understood using H and L energies. The addition of alkyl groups in 3FP3BCH results increment in H-L gap of the molecular structures as the molecule size is increased.

Further, the packing density of the 3FP5BCH increases due to the planarity, and addition of alkyl groups. This stimulates the orbital gap of the molecular systems through which charge transfer

process is accelerated. This acceleration is finally accountable for the nonlinear optical properties.

Global chemical reactivity descriptors (GCRD) have been analyzed in order to realize the link between structures, global chemical reactivity, and stability etc. The hardness of a molecule is related to aromaticity. The GCRD parameters like chemical hardness (η), chemical potential (μ), softness (S), electro negativity (χ) and electrophilicity index (ω) of the molecules based on HOMO, LUMO energies have been given in Table 3. Due to the addition of alkyl groups in 3FP3BCH enhances all the GCRD parameters. The calculated H-L energy gap and chemical hardness values

reveal the chemical stability of titled molecules. The higher energy gap indicates the higher kinetic stability of 3FP5BCH. This is in agreement with the principle of softness-hardness. The hardness of the molecule is justified by the higher energy gap which leads to higher kinetic and thermal stability. Further, the lower energy gap indicates lower kinetic stability and enhanced chemical reactivity as it is energetically probable for the addition of electrons to a high lying LUMO. Moreover, this helps to pull out electrons from a low-lying HOMO. It may be noticed that all the parameters increase with respect to substitution of additional alkyl groups.

Table 3 Calculated values of ionization energy $I=(-E_H)$, electron affinity $A=(-E_L)$, electro negativity $\chi=(I+A)/2$, chemical hardness $\eta=(I-A)/2$, electronic chemical potential $\mu=- (I+A)/2$, electrophilicity index $\omega=\mu^2/\eta$, and softness $S=1/\eta$ of 3FP3BCH and 3FP5BCH molecules using CNDO/S, and INDO/S methods.

Molecule	Method	I/eV	A/eV	χ /eV	η /eV	μ /eV	ω /eV	S/eV^{-1}
3FP3BCH	CNDO/S	9.86	0.96	5.41	4.45	-5.41	6.58	0.22
	INDO/S	8.93	0.11	4.52	4.41	-4.52	4.63	0.22
3FP5BCH	CNDO/S	10.19	1.21	5.70	4.49	-5.70	7.24	0.22
	INDO/S	9.23	0.34	4.78	4.44	-4.78	5.15	0.22

POLARIZABILITY AND NON-LINEAR OPTICAL ACTIVITY

Molecular polarizability values are essential in analyzing the intermolecular electrostatic interaction energies of molecules of no permanent dipole moment. The polarizability helps in assessing the molecular distortion in an electric field. The quantities α_{xx} , α_{yy} and α_{zz} are recognized as the primary values of the polarizability tensor. This property estimates the potency of molecular interactions (e.g., intermolecular long-range induction, dispersion forces, etc.), and the optical properties of a system. The estimated primary polarizability components (α_{xx} , α_{yy} , α_{zz}), isotropic component (α^{iso}) = $(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})/3$, anisotropy $\Delta\alpha = |\alpha_{xx} - (\alpha_{yy} + \alpha_{zz})/2|$, asymmetry $\eta_\alpha = (\alpha_{yy} - \alpha_{zz} / \alpha_{xx} - \alpha^{iso})$ of

3FPnBCH ($n=3, 5$) have been reported in Table 4. The isotropic component of polarizability (α^{iso}) is found to be decreased when the homologue number increases. The molecular polarizability component α_{zz} is larger compared to the rest two components for both molecules. The molecular polarizability components have been found to be decreased with increase in homologue number. The 3FP3BCH has higher polarizability compared to 3FP5BCH.

The higher packing density of 3FP5BCH causes the higher phase stability, and hence the distortion (polarizability) is assumed to be low. Polarizability anisotropy occurs due to the difference between the longitudinal and transverse components of molecular polarizabilities.

Table 4 Principal polarisability components (α_{xx} , α_{yy} , α_{zz}) in a.u., isotropic component (α^{iso}), anisotropy ($\Delta\alpha$), asymmetry (η_α) of the 3FP3BCH, and 3FP5BCH molecules calculated at CNDO/S, and INDO/S levels.

Molecule	Method	α_{xx}	α_{yy}	α_{zz}	α^{iso}	$\Delta\alpha$	η_α
3FP3BCH	CNDO/S	50.64	5.61	68.43	41.56	13.62	-6.92
	INDO/S	51.01	6.61	66.73	41.45	14.34	-6.29
3FP5BCH	CNDO/S	23.32	36.02	63.49	40.94	-26.43	1.59
	INDO/S	23.26	36.22	63.52	41.00	-26.61	1.54

Hence, the total drop in α^{iso} value occurs due to increment in homologue number. The similar trend is followed by asymmetry component, $\eta\alpha$, however, reverse trend has been exhibited by the anisotropy component, $\Delta\alpha$. The higher isotropic polarizability is exhibited by 3FP3BCH to 3FP5BCH implying the actuality that more stability of 3FP5BCH that is in accord with the minimum polarizability principle.

CONCLUSIONS

The following conclusions have been drawn from the present study:

- The increment in temperature scale causes the enough translational freedom for the molecules to slide along the molecular long axis. The phase behaviour of the molecules is estimated to be nematic as higher translational freedom has been observed in planar mode interactions.
- The added alkyl chains in 3FP3BCH cause a blue-shift and the hypochromic effect. Further, reasonable agreement has been noticed in estimation of spectral parameters using both methods.
- The higher energy gap indicates the higher kinetic stability of 3FP5BCH. This is in agreement with the principle of softness-hardness. The higher isotropic polarizability is exhibited by 3FP3BCH to 3FP5BCH implying the actuality that more stability of 3FP5BCH that is in accord with the minimum polarizability principle.

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