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INVESTIGATION OF THE PROPERTIES OF SUPRAMOLECULAR HYDROGEN-BONDED LIQUID CRYSTALS USING FTIR AND THERMAL ANALYSIS TECHNIQUES

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ABSTRACT

This study examines the molecular interactions and thermal characteristics of supramolecular hydrogen-bonded liquid crystals, utilizing FTIR and thermal analysis techniques. Our investigation focuses on the hydrogen-bonded liquid crystal system of p, n-alkoxy benzoic acid: nonyl-p-hydroxy benzoate (nOBA: 9HB), specifically with 'n' values of 6, 7, and 8.The intermolecular interactions between the COOH donor of liquid crystal p-n alkoxy benzoic acid and the OH acceptor of non-liquid crystalline compound nonyl-p-hydroxybenzoate (9HB) result the supramolecular system through hydrogen bonding. The existence and applicability of newly formed systems depend on the strength of the bond formed between the molecules and the stability of the complex system. Here, the molecular vibration method of FTIR and thermal analysis techniques are employed to characterize the supramolecular systems (nOBA: 9HB, where n = 6,7, and 8). Results obtained from this investigation explain how the presence of hydrogen bonds influences the molecular and thermal properties of liquid crystal complexes towards the improvement of device performance and their utility in biological applications.

Keywords: Supramolecular Hydrogen-Bonded Liquid Crystals, Fourier Transform Infrared Spectroscopy, Molecular Interactions, Molecular Polarizability, Phase Transitions.

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INTRODUCTION

Recent studies have highlighted the potential of supramolecular hydrogen-bonded liquid crystals (SMHBLCs) to induce, develop, and stabilize desirable liquid crystal (LC) phase structures for device applications.[1-4] So many authors have reported supramolecular liquid crystals synthesized from combinations of liquid crystalline and non-liquid crystals. Nonetheless, it has been reported that the inclusion of a minimum of one liquid crystalline moiety results in the highest yield in hydrogen-bonded liquid crystals (HBLCs).[5-7] Intermolecular interaction between the compounds in different combinations yields the new liquid crystal complexes via hydrogen bond formation. The formation of hydrogen bonds exerts a remarkable impact on the structural and physical characteristics of supramolecular systems, resulting in properties that are distinct from those of the constituent compounds.[8,9]Here, supramolecular HBLCs p,n-alkoxy benzoic acids: nonyl-p-hydroxy benzoate, abbreviated as nOBA:9HB (where n = 6, 7, and 8) are considered for investigation.[10] The OH group of a non-liquid crystalline compound, nonyl-p-hydroxy benzoate (9HB), and the COOH groups of liquid crystal compounds, p,n-alkoxy benzoic acids (where n = 6, 7, and 8), establish a hydrogen bond to produce the SMHBLCs. Generally, the fundamental task involved in any newly formed hydrogen-bonded system is the conformation of the hydrogen bond in the supramolecular system, and this can be done through Fourier transform infrared (FTIR) spectral analysis.[11-13]FTIR spectrum data can be used to determine the vibrational frequencies of functional groups that are involved in the formation of hydrogen bonds. The parameters measured from these vibrational frequencies of the molecules give information about the strength of the bond formed between the compounds.[14,15] Such parameters are molecular polarizabilities, polarizability anisotropy, and related

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parameters like force constant, bond length, etc.[11-13] All these are important parameters for characterizing the molecular interactions of newly formed liquid crystalline complexes. Numerous experimental and theoretical investigations have been posited to examine the intermolecular interactions of liquid crystals.[16-18] But using these methods, most of the work is reported on liquid crystalline materials, and less work is reported for supramolecular hydrogen-bonded liquid crystals. This generates great research to study the molecular polarizabilities and their anisotropy of the SMHBLCs using the molecular vibration method of FTIR. The Molecular Vibration Method accurately reflects any minor alterations in intermolecular forces resulting from modifications in the chemical environment through the precise depiction of their force constants and vibrational frequencies.[11-16]Therefore, a systematic investigation for molecular studies is done by calculating the intermolecular interaction parameters like force constant, bond length, molecular polarizabilities, and polarizability anisotropy from the Fourier Transform Infrared (FTIR) spectra. Another basic thing for any newly formed liquid crystalline material is the identification of phase transitions and the stability of the mesophase (liquid crystalline phase). Thermal analysis techniques: Polarizing Optical Microscope (POM), and Differential Scanning Calorimetry (DSC) are employed for this purpose.[19] Results obtained from this investigation explain the impact of the existence of hydrogen bonding within liquid crystal complexes on the efficacy of systems with regard to their properties and applicability in biological contexts.

EXPERIMENTAL

The chemical compounds p,n-alkoxy benzoic acid (nOBA, where n = 6, 7, and 8), and nonyl-p-hydroxy benzoate (9HB) were procured from Frinton Laboratory, New Jersey, USA. In this study, an equimolar (1:1) ratio of the liquid crystalline compound p-n alkoxy benzoic acids (nOBA) was combined with the non-liquid crystalline nonyl-p-hydroxy benzoate (9HB) to synthesize novel liquid crystal complexes, denoted as (nOBA: 9HB, n = 6, 7, and 8).[10] The Fourier-transform infrared (FTIR) spectra of the individual compounds and their complexes were recorded using an Alpha-model Bruker Infrared Spectrometer. Differential scanning calorimetry (DSC) was performed on a DSC Q20 V24.2 Build 107 universal V4.5 TA instrument (at a heat or cool rate of 5°C/min). The textures of the samples were observed using an SD-Tech Polarizing Optical Microscope with a hot stage and camera attachment.[19,20] The theoretical framework underpinning the present investigation is elaborated on in the subsequent section.

Theory

The modification of the chemical environment surrounding a bond within a molecule initiates the production of new molecules and complex systems that display unique structural and physical properties. The existence and applicability of newly formed systems depend on the strength of the bond formed between the molecules and the stability of the newly formed complex system. Intermolecular interactions and thermal studies of LCs are helpful in getting a better understanding of these kinds of liquid crystal complexes. Here, the molecular vibration method of FTIR and different thermal analysis techniques (POM, DSC) are employed for this purpose. Parameters like force constants and bond lengths are explained in.[11-15]

Molecular Vibration Method

The molecular vibration method of FTIR is used to study the molecular interactions of supramolecular systems using molecular polarizability and its polarization anisotropy. These parameters are very sensitive to shifts in the vibrational frequencies of the bonds.[16-18]Using the force constants and mean amplitudes of vibration, longitudinal and transverse bond coefficient values, and the mean molecular polarizability of SMHBLCs are measured from the following equation:

$$\text{Mean molecular polarizability } \alpha_M = \left[\frac{\sum n_i (b_L + 2b_T)}{3} \right] \quad (1)$$

Where 'b_L' and'b_T' are the longitudinal and transverse bond coefficients,'n_i' is the number of bonds in a molecule. 'b_L +2 b_T' values for different vibrational frequencies of bonds are calculated from the mean amplitude of vibration '$\sigma^{1/2}$'.

$$(b_L + 2b_T) = \mathrm{CP^j j^{nr}} \sigma^{1/2} \quad (2)$$

The terms involved in the above equations are explained in the.[12,13]

The equation relating longitudinal (b_L) and transverse (b_T) bond polarizabilities with stretching force constant (K) is[17]

$$b_L - b_T = A\left[(X_1X_2)^{1/2}\left(\frac{aN}{K-b}\right)^{2/3}\right]^S \quad (3)$$

$$S = \frac{K}{3b-2K} \quad (4)$$

The electro-negativities of the atoms involved in the bond of length (r), denoted as X1 and X2, and the bond order N are the parameters under consideration. The constants 'a' and 'b' are Gordy's coefficients. A is characteristic of the bond.[16-18] The individual bond polarizability coefficients (b_L and b_T) are obtained from equations (2) and (3).

Polarizability Anisotropy

Molecular Polarizability anisotropy of liquid crystal $\Delta\alpha = \alpha_{\square} - \alpha_{\perp}$ (5)

Where '$\alpha_{\square}$' is parallel polarizability,' $\alpha_{\perp}$' is perpendicular polarizability.

Using Mean molecular polarizability (α_M), Parallel and Perpendicular polarizabilities ('$\alpha_{\square}$' and $\alpha_{\perp}$), Polarizability anisotropy can be written as [16]

$$\alpha_{\square} - \alpha_{\perp} = \frac{3}{2}(\alpha_{\square} - \alpha_M) \quad (6)$$

The polarizability component that is aligned with the molecular axis of a given molecule can be expressed as follows:[12]

$$\alpha_{\square} = \sum \bar{\alpha}_{\square} \cos^2\theta + \sum \bar{\alpha}_{\perp} \sin^2\theta \quad (7)$$

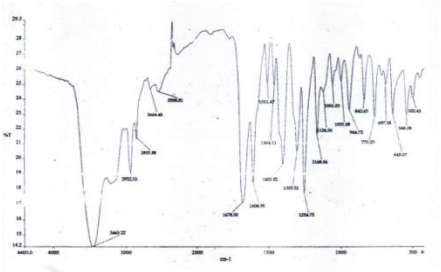
The angle "θ" represents the angle between a bond and the molecular axis, while "$\bar{\alpha}_{\square}$" and "$\bar{\alpha}_{\perp}$"denote the parallel and perpendicular bond components of the polarizability, respectively. In instances where the molecular structures of certain substances have not been confirmed, it is assumed that the bond angles are 120^0.[16,17] From the parallel and perpendicular polarizabilities obtained from equations (6 and 7), polarizability anisotropy $\Delta\alpha$ can be estimated.

RESULTS AND DISCUSSION

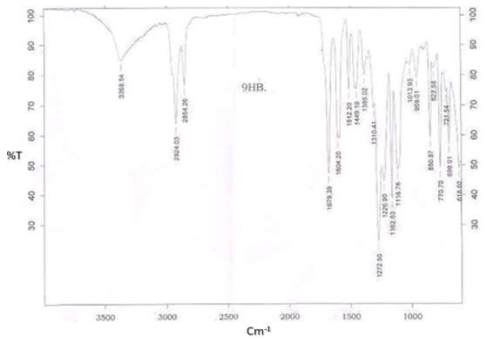
The molecular interactions and thermal characteristics of synthesized supramolecular hydrogen-bonded liquid crystals are studied using FTIR, POM, and DSC techniques. Intermolecular interactions involved in the formation of SMHBLCs via hydrogen bond formation are studied using the molecular vibration method of FTIR spectral data.

Molecular Interaction Studies From FTIR

FTIR spectra of p-n alkoxy benzoic acid (nOBA, where n=6,7, and 8) and nonyl-p-hydroxy benzoate (9HB), and supramolecular systems (nOBA:9HB, where n=6,7, and 8) were recorded at room temperature in solid (KBr) and are shown in Fig.-1. As a representative case, IR spectra of 7OBA, 9HB, and 7OBA:9HB samples are shown.



(a)



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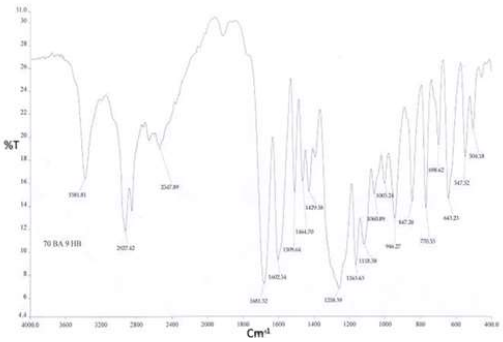


(c)

Fig.-1: FTIR Spectra of (a) 7OBA;(b) 9HB;(c) 7OBA: 9HB.

Table-1 presents the IR frequency assignments for various modes of vibration in both pure and complex systems.

Table-1: IR Frequency Assignments (cm^{-1})for Different Modes of Vibrations of nOBA, 9HB, and nOBA:9HB (n=6,7, and 8)

Compound	O-H	C-H	C-O	C=O
6OBA	3437.46	2933.16	1296.57	1691.62
7OBA	3463.22	2932.33	1305.54	1678.5
8OBA	3441.83	2930.91	1297.99	1684.97
9HB	3369.54	2854.26	1162.53	----------
6OBA:9HB	3382.87	2926.12	1280.8	1682.79
7OBA:9HB	3381.81	2927.42	1258.39	1681.32
8OBA:9HB	3381.98	2925.55	1280.26	1684.33

In pure p-n-alkoxy benzoic acids, the O-H vibrational band occur around 3400 cm^{-1} - 3500 cm^{-1}, C=O, C-O vibrations occur around 1670 - 1691 cm^{-1}, 1290-1310 cm^{-1}.The other symmetrical stretching and bending modes of frequencies confirm the dimeric nature of alkoxy benzoic acid. In pure 9HB, the vibrational band corresponding to O-H stretching exists around 3369.54cm^{-1}. SMHBLCs formed from the non-mesogenic compound 9HB; the dimers of alkoxy compounds separated out as monomers,as evidenced by the shifts in the vibrational frequencies, which show that, a hydrogen bond is forming. It is invoked on the basis of bathochromic shifts and hypsochromic shifts in the vibrational frequencies of functional groups (C-O,C-H,C=O,O-H). The infrared spectra of SMHBLCs nOBA: 9HB exhibit robust and intense bands attributed to the (C=O, C-O) modes of the benzoic acid moiety, located at approximately 1684.33 cm^{-1} and 1258-1280 cm^{-1}, respectively. This strongly implies that, after complexation, the nOBA moieties reside in a monomeric form.Thebathochromic shifts in the vibrational frequencies of (C=O) acid are ~9 cm^{-1} and (C-O) acid is in the range of ~10- 47cm^{-1}, and a characteristic peak (O-H) of acid associated with high intensity is around 3382cm^{-1}, which confirm the formation of hydrogen bonds in supramolecular systems. The observed shifts in the C=O and C-O stretching modes of supramolecular hydrogen-bonded liquid crystals (SMHBLCs) towards the lower frequency side of the spectrum can be attributed to the hydrogen bonding interaction between the C=O group of benzoates and

the hydroxyl group. The nature of the shifts also describes the strength of bonds in supra-molecular systems. Here, this can be done by measuring molecular interaction parameters: force constant, bond length, and molecular polarizabilities since they are very sensitive to these shifts in the vibrational frequencies of functional groups. The parameter values of the pure (nOBA, 9HB) and complex systems nOBA:9HB (where n=6,7,and 8) are tabulated.

Table-2:Force constants (N/cm) of vibrational modes of nOBA, 9HB, and nOBA:9HB (n=6,7,and 8)

Compound	O-H	C-H	C-O	C=O
6OBA	0.659	0.506	0.678	1.155
7OBA	0.669	0.506	0.687	1.137
8OBA	0.661	0.505	0.679	1.154
6OBA:9HB	0.639	0.504	0.662	1.143
7OBA:9HB	0.637	0.503	0.645	1.14
8OBA:9HB	0.637	0.503	0.661	1.141

Table-3: Bond Length (A^o) of Vibrational Modes of nOBA, 9HB, and nOBA:9HB (n=6,7, and 8)

Compound	O-H	C-H	C-O	C=O
6OBA	2.954	3.225	2.9	2.45
7OBA	2.939	3.226	2.91	2.46
8OBA	2.951	3.227	2.92	2.45
6OBA:9HB	2.985	3.232	2.95	2.56
7OBA:9HB	2.986	3.23	2.98	2.56
8OBA:9HB	2.986	3.231	2.95	2.55

Tables-2 and 3 give the force constant and bond length values of vibrational bands of the pure and complex systems involved in bond formation. The force constant of the vibrational modes of nOBA: 9HB are in the range of 0.638 to 1.143, and bond lengths are in the range of 2.5-3.2A^o, which represents the strength of the bond as moderate.[12-14]Generally, vibrational modes that have large force constants and low bond length values are strongly involved in bonding.[13]In the case of these supra molecular systems (nOBA:9HB, where n= 6,7, and 8), there is no significant difference in the magnitude of the intermolecular interaction parameters. Almost all are in the same range but have different values from the pure systems. This is due to the fact that the hydrogen bond in the supramolecular systems is formed from the strong electrostatic interactions of the pure systems, which confirms strong molecular interactions in supramolecular systems 6OBA: 9HB, 7OBA:9HB, and 8OBA: 9HB.The mean molecular polarizability(α_M) and polarizability anisotropy ($\Delta\alpha$) of given supramolecular systems are computed from the molecular vibration method using equations (1) - (7).This method gives an empirical relation for the computation of parallel and perpendicular molecular polarizabilities ($\alpha_{\square}$ and $\alpha_{\perp}$) from mean molecular polarizabilities, force constant, bond order, and amplitude of vibration.[16-18]The mean molecular polarizability of pure and complex systems is given in Table-4.

Table-4: Mean Molecular Polarizability (α_M*10^{-25} cm^3), values of Bond Polarizability Coefficients (b_L*10^{-25} cm^3 and b_T*10^{-25} cm^3) of nOBA and nOBA:9HB (n=6,7, and 8)

Compound	Molecular Polarizability	Polarizability Coefficients	
	α_M	b_L	b_T
6OBA	45.5	55.4	39.2
7OBA	49.7	60.8	43
8OBA	54	66.3	46.7
6OBA:9HB	102.2	128	88.7
7OBA:9HB	106.8	134	92.6
8OBA:9HB	114.3	136	96.2

From Table-4, it was observed that 'α_M' values of complex systems are high compared to those of pure systems. This is due to the fact that the vibrational modes involved in hydrogen bond formation have good contributions towards molecular polarizability. Eventually, they sum up, leading to a significant

increase in the mean molecular polarizability of the complex systems, which increases with increasing chain length n = 6 to 8.By solving equations (2,4), the longitudinal and transverse bond polarizability coefficients (b_L and b_T) of the vibrational bands involved in the bond formation are also computed. The values of 'b_L and b_T' also increase with increasing carbon atoms. This is also shown in Table-4.Using equations (5, 6, and 7) molecular polarizabilities ($\alpha_{\square}$and $\alpha_{\perp}$) and polarizability anisotropy ($\Delta\alpha$)of complexes are computed and presented in Table-5. Like mean polarizability, molecular polarizabilities ($\alpha_{\square}$ and $\alpha_{\perp}$) also increase with increasing chain length, n= 6 to 8.However, the polarizability anisotropy shows even odd behavior against the mean polarizability with alkoxy chain length.

Table-5: Molecular Polarizabilities ($\alpha_{\square}$ *10^{-25} $cm^3$and $\alpha_{\perp}$*10^{-25} cm^3) and Polarizability Anisotropy ($\Delta\alpha$*10^{-25} cm^3) of nOBA and nOBA:9HB (n=6,7, and 8)

Compounds	$\alpha_{\square}$	$\alpha_{\perp}$	($\Delta\alpha$)
6OBA	49.92	43.2	6.65
7OBA	54.8	47.1	7.61
8OBA	59.72	51.1	8.58
6OBA:9HB	114	95.8	18.9
7OBA:9HB	119	100.2	19.7
8OBA:9HB	124	109.1	14.9

In SMHBLCs, the contributions towards the mean polarizability of systems are derived from the covalent bond electrons in the alkoxy chain, whereas for polarizability anisotropy, they mainly come from the core contribution.Therefore,variations in the mean polarizability values increase with increasing chain length compared to variations in the Polarizability anisotropy values.Also,the effect on the stability of complex systems due to molecular polarizabilityis irregular since the waggling of the end segment of the alkoxy chain is more disordered than the core, and molecular polarizability depends on the molecular size, electron density, bond length, shape, and mass.

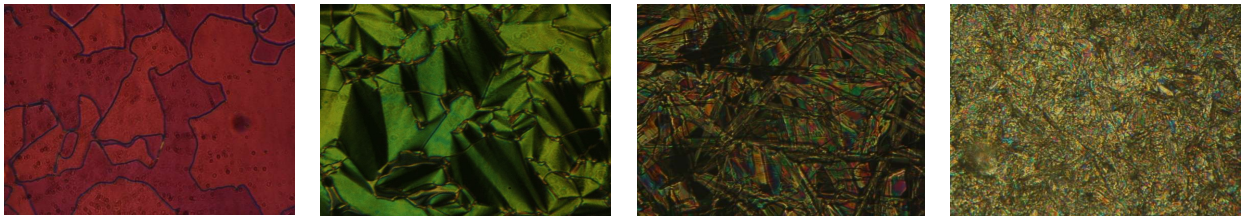
Thermal Studies

Thermal analysis studies of SMHBLCs (nOBA: 9HB, where n=6,7, and 8) are carried out using Polarizing Optical Microscope and Differential Scanning Calorimetry techniques. The textures of the liquid crystals and their complexes are recorded using POM. Compounds 6OBA, 7OBA, and 8OBA exhibit the enantiotropic nematic phase and, 7OBA, 8OBA exhibit the enantiotropic Smectic C phase. Hydrogen bond formation due to the complexation of nOBA and 9HB quenches the nematic phase, (of 6OBA, 7OBA, and 8OBA) the smectic C phase (of 7OBA, 8OBA) and induces the Smectic G phase for the SMHBLCs - nOBA: 9HB(where n=6,7 and 8). Whereas in 8OBA:9HB, it induces the Crystal 2 phase in addition to the Smectic G phase.[21,22]They are shown in Fig.-2.

The aromatic core of nOBA (where n=6, 7, and 8) and 9HB, which possess terminal chains, exhibits a propensity to densely arrange the molecules in a layered structure. This arrangement leads to the formation of the Smectic G phase and the Crystal 2 phase in 8OBA:9HB. The mesophase behavior of the resulting esters (nOBA: 9HB) can be correlated with the length of the alkoxy chain in the esterified nOBA molecules (n=6, 7, and 8). Esterification of the nOBA molecular structures with 9HB, which bears a terminal alkoxy chain, is responsible for this modification. The transition temperatures of the SMHBLCs are recorded using the POM technique. These phase transition temperatures are evaluated with DSC measurements. They are shown in Table-6. As a representative case, DSC thermograms of 7OBA: 9HB and 8OBA: 9HB are shown in Fig.-3.

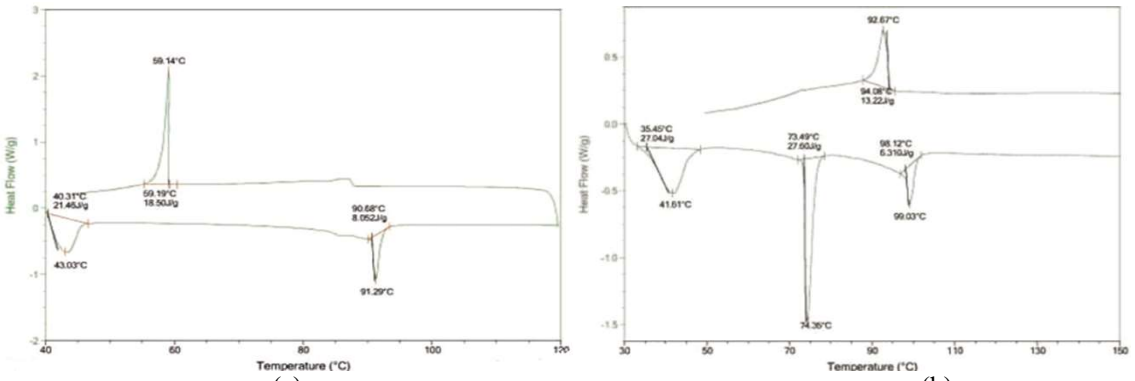
From Table-6, it was observed that the liquid crystalline range of SMHBLCs is about (28^0C – 58^0C). The 6OBA:9HB complex exhibits a mesophase range of 28^0C which is low compared to the other supra molecular systems 7OBA:9HB (46.1^0C), 8OBA:9HB (57.9^0C), and pure systems (48.6^0C,55^0C,41.1^0C).The liquid crystal complexes of nOBA:9HB exhibit the even-odd effect during the Cr – Smectic G – Isotropic phase transitions, with higher transition temperatures corresponding to even numbers.[23] The flexible end chains of nOBA molecules undergo modification based on the value of 'n' in its pure form. In hydrogen-bonded liquid crystals, one end is fixedly connected to the hydroxyl benzoate

with a chain length of nine (9) and the other end is coupled to a changeable flexible chain length 'n'. These supramolecular systems are characterized by the formation of the Smectic G phase attributed to the benzoate family, which reduces transition temperatures to maintain a layered arrangement.The influence of flexible alkoxy chain components and other steric factors like size, and shape, induces the Smectic G and the interruption of one phase by other phases.[24]



(a) (b) (c) (d)

Fig.-2: Textures of Liquid Crystalline Phases (a) Nematic Phase of nOBA(n=6-8); (b) Smectic C Phase of nOBA (n=7,8); (c) Smectic G Phase of nOBA: 9HB (n=6-8); (d) Crystal 2 Phase of 8OBA:9HB.



(a) (b)

Fig.-3: DSC Thermograms of (a) 7OBA:9HB;(b)8OBA:9HB

Table-6: Phase Transitions and their temperatures of p,n-alkoxy Benzoic Acid (nOBA) and Liquid Crystal Complexes p,n-alkoxy Benzoic Acid: nonyl -p–hydroxy Benzoates (nOBA:9HB, where n=6,7,and 8)

Compound	Phases	Temperatures of phase transition (°C)	
		POM	DSC
6OBA	Cr – N – I	101.9 – 150.5	106.8- 148.8
7OBA	Cr – SmC – N – I	89.5 – 97.5 – 144	87.62 – 95.9 – 147.8
8OBA	Cr – SmC – N – I	95.1 – 102.4 – 136.2	91.1 – 100.9 – 137.1
6OBA:9HB	Cr – SmG – I	72.3 – 101.0	72.12 – 103.83
7OBA:9HB	Cr – SmG – I	42.1 – 88.2	43.03 – 91.21
8OBA:9HB	Cr – Cr2 – SmG – I	38.3 – 77.67 – 96.20	41.61 – 74.36 – 99.03

(Cr – Crystal, Cr2 – Crystal 2, SmG - Smectic G, SmC- Smectic C, I- isotropic)

Therefore, decreasing transition temperatures and the stability of hydrogen bonding depend on the structural property relationship, chain length, molecule size, and position of terminal substituents. The liquid crystalline stability of the complex systems is also proved from the calculation of phase transition activation energies which uses the DSC measurements. Activation energy is a barrier to liquid crystalline phase transformation, and it changes the molecular arrangement with respect to temperature. Here, activation energies are calculated from the Ozwa method[25,26] and are presented inTable-7.

From Table-7, it was observed that the activation energies for pure compounds are high compared to those for hydrogen-bonded systems. For pure and supramolecular systems (nOBA, nOBA:9HB, where n = 6, 7, and 8), the activation energies are high for the liquid crystal phase (Smectic G) - isotropic phase transition compared to the crystalline-liquid crystal phase. The heightened activation energy denotes a significant energy threshold for the phase transformation process. This implies that complex systems also maintain liquid-crystalline phase stability like pure systems.

Table-7: Activation Energy (kJ/mole) of nOBA, nOBA:9HB (where n= 6,7, and 8)

Compounds	Phases	Activation energies
6OBA	Cr – N – I	75.15 – 104.31
7OBA	Cr – SmC – N – I	62.96 – 67.20 – 104.31
8OBA	Cr – SmC – N – I	64.11 – 70.59 – 97.06
6OBA:9HB	Cr – SmG – I	50.64 – 72.80
7OBA:9HB	Cr – SmG – I	30.12 – 64.11
7OBA:9HB	Cr – Cr2 – SmG – I	29.12 – 52.15 – 69.89

(Cr – Crystal,Cr2- Crystal 2, SmG - Smectic G, SmC- Smectic C, I- isotropic)

Results obtained from this investigation show that intermolecular interactions between the nOBA and 9HB yield strong and stable liquid crystalline complexes with increasing alkoxy chain lengths (n = 6 to 8). The supramolecular system 8OBA:9HB is more stable with strong molecular interactions compared to 6OBA:9HB and 7OBA:9HB. Hydrogen bond formation in these supramolecular liquid crystals influences the molecular and thermal properties of the material. This leads to an improvement in the material performance of the applications. In general, benzoic acids and their substituents are used as antibiotics and preservatives in the pharmaceutical industry. Here, SMHBLCS synthesized from these benzoic acid derivatives is useful for biological applications.[27] The high molecular polarizabilities and moderate bonding nature of these complexes make them good binding nature with suitable targets for biological species. The interaction between liquid crystals and biological entities results in a perturbation of the molecular arrangement within the liquid crystal system.As a result, the vibrational frequencies, molecular polarizabilities, molecular arrangement, and other physical properties like transmitted intensities, refractive index, birefringence, etc. of complex systems will change. Analysis of these properties will be useful for the identification of targeted species and the design of new drugs and sensors for biological applications.

CONCLUSION

The molecular interactions and thermal analysis studies of the supramolecular hydrogen-bonded liquid crystals nOBA:9HB (where n = 6, 7, and 8) are successfully investigated using FTIR and thermal analysis techniques POM and DSC. Intermolecular interactions between the nOBA and 9HB form strong and stable complex systems with increasing alkoxy chain lengths (n = 6 to 8). These complex systems have significant liquid crystalline properties and will be useful for the fabrication of devices in biological applications.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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REFERENCES

1. J. M. Lehn, *Angewandte Chemie International Edition in English*,**27**, 89(1998).
2. Bing Liu, Tao Yang, Xin Mu, Zhijian Mai, Hao Li, Yao WangandGuofu Zhou, *Nanomaterials*, **11**, 448(2021), https://doi.org/10.3390/nano11020448.
3. G. Sangameswari, N. P. S. Prabu, M. A. Mohan, *Liquid Crystal*, **45(3)**, 1(2018), https://doi.org/10.1080/02678292.2017.1342145.
4. M. Hagar, H. A. Ahmed, R. B. Alnoman, M. Jaremko, A. H. Hamid Emwas, S. Sioud and K. A. Abu Al-Ola, *Frontiers in Chemistry*, **9**, (2021), https://doi.org/10.3389/fchem.2021.679885
5. M. Muni Prasad, M.L.N. Madhu Mohan, P.V. Chalapathi, A.V.N. Ashok Kumar, D. M. Potukuchi, *Journal of Molecular Liquids*, **207**, 113(2015), https://doi.org 10.1016/j.molliq.2015.03.025
6. P. Y. W. Dankers, E. W Meijer, *Bulletin of the Chemical Society of Japan*, **80**, 2047(2007) https://doi.org/10.1246/bcsj.80.2047.
7. T. Kato, M. Fukumasa, J. M. J. Fretchet, *Chemistry of Materials*,**7**, 368(1995).
8. C. M. Paleos, D. Tsiourvas, *AngewandteChemie International Edition in English,***34**, 1696(1995).
9. Virgil Percec, *The Royal SocietyA*, **364**, 2709(2006), https://doi.org/10.1098/rsta.2006.1848.
10. S. Sreehari Sastry , C. Nageswara Rao , T. Vishwam , K. Mallika , B. Gowri Sankara Rao, and Ha Sie Tiong, *Research Journal of Physical Sciences,***6(1),**1(2013).
11. R.M. Silverstein, F.X. Webster, Spectroscopic identification of organic compounds, John Wiley and Sons, New York, (2004).
12. http://www.umsl.edu/~orglab/pdffiles/ir.pdf/
13. P. V. Raut, P. P. Choudhari, *Rasayan Journal of Chemistry,***16(1)**, 14(2023). http://doi.org/10.31788/RJC.2023.1618170
14. N. Andalia, M.N. Salim , N. Saidi , M.Ridhwan and U. Balqis, *Rasayan Journal of Chemistry,***16(1)**, 9(2023), http://doi.org/10.31788/RJC.2023.1618051
15. C.P. Sherman Hsu, 2000, Infrared Spectroscopy,in: F.A. Settle (Eds.), In Handbook of instrumental techniques for analytical chemistry; Prentice Hall PTR: Upper Saddle River, New Jersy, pp. 247–283, https://doi.org/10.1080/10826079808006889
16. Y. N. Murthy, *Acta Physica Polonica A*, **91(6),** 1069(1997), https://doi.org/10.12693/APHYSPOLA.91.1069.
17. Dudumoni Bhuyan, Ph.D.Thesis, Department of Physics, North Eastern Regional Institute of Scienceand Technology (NERIST), Nirjuli, Arunachal Pradesh, India, 2013.
18. L. Jun, Ph.D.Thesis, Department of Optics and Photonics, University of Central Florida, Orlando, Florida, (2019).
19. D. Demus and L. Richter, Textures of Liquid Crystals, Verlag Chemie, New York, (1978).
20. C.N. Rao, K.J. Rao, Phase Transition in Solids-An Approach to the Study of the Chemistry and Physics of Solids, McGraw-Hill, New York, (1978), https://doi.org/10.1038/275258c0
21. C.Ravi Shankar Kumar, A.Jha, S.Sreehari Sastry, *Journal of Non- crystalline Solids*, **356**, 334(2010), https://doi.org/10.1016/j.jnoncrysol.2009.11.036
22. P.Swathi, P. A. Kumar, V. G. K. M. Pisipati, *Molecular Crystals Liquid Crystals*, **365**, 523(2001), https://doi.org 10.1080/10587250108025332
23. Chen dan-mei, Dong Yan-ming, Shen Bing-Xing, Yang Xue-hui,Liyan-jie, Hu Xiao-lan, *Chemical Research Chinese Universities*,**25**, 579(2009).
24. M.Muniprasad, M.Srinivasulu, P.V.Chalapathi, D.M.Potukuchi, *Molecular Crystal Liquid Crystal*s, **557,** 102(2012),https://doi.org/10.1080/15421406.2011.636662
25. Mustafa Okumuş, ŞükrüÖzgan and Süleyman Yılmaz, *Brazilian Journal of Physics,***44**, 326(2014), https://doi.org 10.1007/s13538-014-0217-7
26. Pere Roura, and Jordi Farjas, *Journal of Materials Research,***24(10)**,3095(2009), https://doi10.1557/jmr.2009.0366.
27. A. V. Doshi, C. G. Joshi,V. R. Patel, *Der Pharma Chemica*, **3(5)**, 191(2011).

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