



RESEARCH ARTICLE

Molecular Dynamics of Mesogenic p-n-alkoxy benzoic acid

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Abstract

The article presents novel attempt on the molecular moment of liquid crystalline molecule that arises due to orientation and position. In particular orientation originated from rod like that exhibiting nematic phases due to its symmetrical structure where the centre of gravity of centre of molecule coincides unlike the positional order exhibits smectic C phase. Homologous series of molecule the p-n-alkoxy benzoic acid with carbon or alkyl chain length extending from propoxy to dodecyloxy is considered. The molecular dynamics is studied in interpretation of its rotational kinetic energy, thermal energy, Moment of inertia, critical velocity and its dipole moment. Studies reveal that the moment of Inertia varies inversely with critical velocity that conserves angular momentum and further observed that polarity is unaffected with increase in chain length. Results of calculations using this type of modeling reveal interesting features that are in agreement with experimental results of concerned systems.

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Introduction

Liquid crystals gained extraordinary importance due to its technological importance due to its anisotropic nature with specific characteristic of self assembling. A number of phase transitions exist in liquid crystals nematics gained importance due to its short range positional order and smectics with long range positional order. Normally the texture is characterized due to its molecular arrangement, due to its interactions and further breaking the molecular packing with temperature as external agent termed as thermotropic liquid crystals. Texture analysis has employed as a primary tool for characterization of different liquid phases. Computational studies of these liquid crystal molecules that are realized as mechanical systems [1-2] are desirable and efficient to obtain its features. This article provides a quantitative model [3-4] to understand the observed experimental results [5] that are nematic and smectic in a mesogenic groups along with segments in flexible chain are realized. Computational studies [6-8] of these are important to understand molecular dynamics which are feasible and desirable for modeling are simple and efficient that explores the features that are typical for intermolecular interactions. The approach is attributed with the key aspect that the centers are coincided that reveals the orientation order of nematics that are spherical at higher temperatures and further thermal stability lead to perform modeling. Extensive studies [9-13] are performed in experimental and novel theoretical techniques [14-17] still required to explore the properties of this interactive liquid crystal that are in ambient temperature range. The aim of this article is to analyze critically for its implication of supramolecular structures.

Materials and Methods

Frinton laboratories supplied the liquid crystalline samples the p-n-alkoxy benzoic acid with chain length extending from propoxy to dodecyloxy. These are used as such without any purification and highly stable due to temperature variations. These exhibit both the nematic and smectic phases before reaching isotropic state from its crystalline state. The textural observations were realized by using Hertel Reuss super-pan II polarizing optical microscope (POM) equipped with optical display (DP10) at scan rate of 0.1° C per minute. The theoretical attempt to study the

dynamics of liquid crystal is performed by structural optimization using Avogadro version 1.0 in z-matrix format further estimated by Gaussian03v for dynamic parameters of molecule that correlates the liquid crystal texture

Results

The formulation of the problem is initiated in determining the moment of inertia, critical velocity, dipole moment, rotational kinetic energy and the thermal energy determined from transition temperatures. Functional molecules responsible for formation of textures are attributed with structure as indicated in figure 1 for molecules with representative nonyloxy benzoic acid with molecular formula $C_{16}H_{24}O_3$ with red indicating oxygen, grey carbon and white indicating hydrogen. Table 1 shows a compilation of molecular parameters of supramolecular self-assembled materials and their textures exhibit that mesophase order is ubiquitous in functional and structural materials. All the members of the series exhibit the nematic phase along with strong positional order that allows materials to flow in the higher members from 7 to 12 of the homologous series above its crystalline state. The highest thermal span of nematic to crystal is observed in the molecules with flexible chain ($n \geq 7$) to possess long range positional order altering the order of transition to second order before transforming to crystalline state. Molecular behavior described by parameter exhibit abrupt variation in moment of inertia from chain length 7 with additional phase. The moment of inertia in figure 2 and critical velocity figure 3 as function of chain length exhibited inverse relation that reflects the molecular moment about the director. Dispersive forces and dipole moments are responsible for mesophase stability with an approximate of 6 debye units in entire chain length differed by small amount in $n=6$ and 12 that arises due to induced dipole moments. The transition temperatures are high with absence of smectic phase where intermolecular forces play dominant role.

Discussion

An accepted fact is that constituent molecules restricted to rotate around its axis resulted in orientational order and some molecules with no rotation results in positional orders form a number of liquid crystalline phases. The molecules tend to have the same alignment towards director on further cooling their positional order is increased before transforming to crystalline state. The mesogenic phases are characterized with permanent dipoles and polarizability with multiple bonds along their axis with terminal group associates nematic phase in entire homologous series with smectic phase with long chains

The relationship between phase structure and geometric structure is the focus of paper that explores to study the dynamic behaviour of molecules that terminate with flexible chains. Molecular polarizabilities and their anisotropy explore inherent molecular properties that arise due to intermolecular interaction energies. The transition from nematic to isotropic transition temperatures in lower chain and nematic to smectic and to isotropic is observed are explained with number of models. However explanation with molecules as rotors was explained with significant way. Liquid crystal molecules with low molecular weight have small moment of inertia exhibiting elevated temperatures. The phase behavior and properties of these liquid crystals depend strongly on the length of flexible chain. Even odd effects are observed in parameters like critical velocity and moment of inertia. Textures are unaltered with increase in chain length with sudden inclusion of smectic C phase from $n > 6$ further with transition temperatures increased with increased chain length. The molecules exhibited polarizabilities that are distributed anisotropically in space are almost identical with increase in chain length.

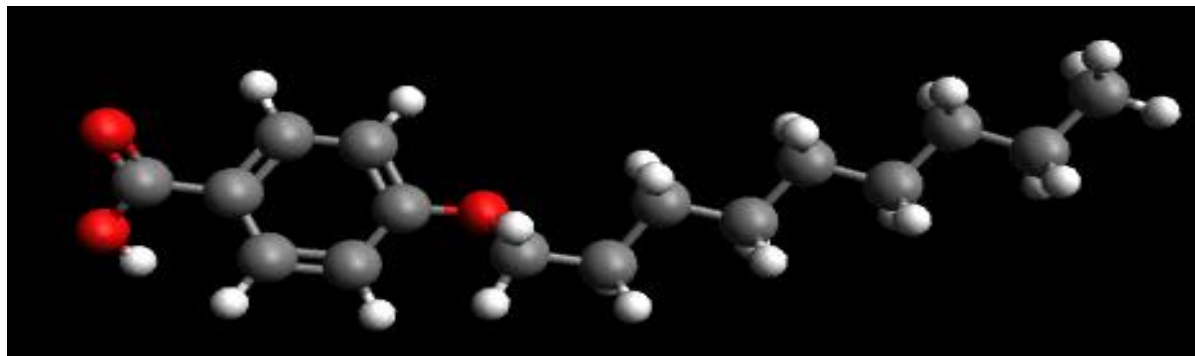


Fig.1. Molecular Structure of Nonyloxy benzoic acid

Table 1: Molecular Parameters of Textures

Chain Length	(I) x 10 ⁻⁴⁷	Phase Variant	(w) x10 ¹¹ rad/sec	T °C	Dipole Moment (μ) Debye
3	3140	N	32.47	154.9	6.52
		C	-	-	
		Crystal	30.43	145.2	
4	5320	N	25.78	160.1	6.75
		C	-	-	
		Crystal	23.69	147.1	
5	5440	N	24.11	151.4	6.01
		C	-	-	
		Crystal	19.73	123.9	
6	7023	N	21.55	153.8	5.65
		C	-	-	
		Crystal	14.84	105.1	
7	11053	N	16.40	146.8	6.85
		C	10.98	98.3	
		Crystal	10.25	91.8	
8	11551	N	16.12	147.5	6.51
		C	11.13	101.9	
		Crystal	10.68	97.8	
9	13291	N	14.56	142.9	6.93
		C	11.19	117.1	
		Crystal	9.82	94.5	
10	19923	N	11.51	138.3	6.87
		C	9.62	115.6	
		Crystal	8.07	97	
11	19490	N	11.36	135.1	6.09
		C	10.47	124.5	
		Crystal	7.026	83.5	
12	23218	N	10.57	137.2	5.85
		C	9.78	128.9	
		Crystal	7.33	95.1	

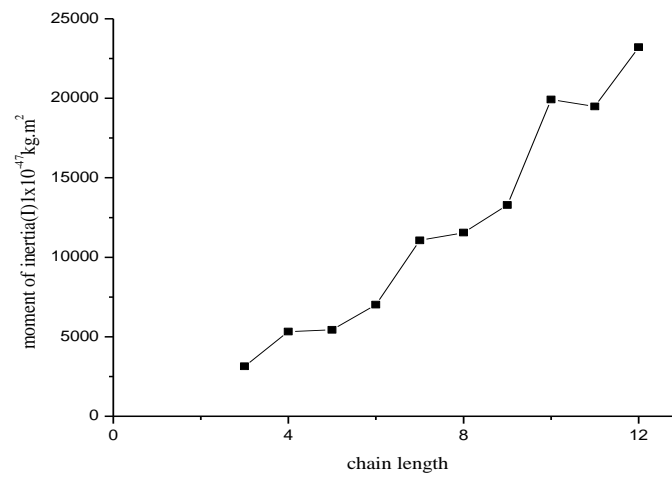


Fig.2. Dependence of Moment of Inertia on chain length

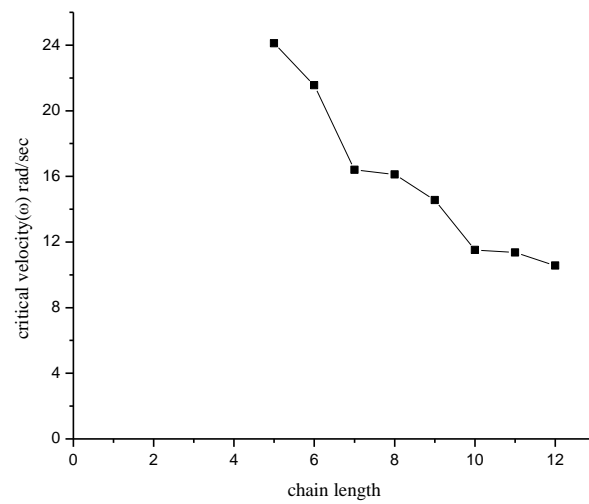


Fig.3. Dependence of Critical velocity on chain length

Conclusions

The optimization of these liquid crystals was performed by computing the significant parameters responsible for formation of liquid crystalline phases that are consistent in formation of supramolecular structures with self assembly. The phases are characterized with critical parameters reveal that rotational parameters influence largely with greater chain length in formation of both nematic and smectic phases with decreased transition temperatures altering the order of transition from first order to second order due to polydispersity. The computational analysis performed systematically explains the formation of liquid crystalline textures with fact that dipole moments are remaining invariant in formation of textures. Moment of inertia which encodes geometrical characteristics of molecules exhibit increasing trend with chain length. This model was explained accurately and successfully with the experimental results that validates the theoretical model. The present work seeks to describe structure, dynamics, and processes found in nature's mesophases using well-established LC models.

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