International Journal of Environmental Sciences
ISSN: 2229-7359
Vol. 11 No. 20s, (2025)
https://theaspd.com/index.php/ijes

Effect of activation energy on the mobility of free charge carriers in liquid crystals' reentrant nematic and smectic phases of liquid crystals

T.N. Govindaiah[1], V. Siva prasad[2]
[1,2]Department of Physics, Government First Grade College, Channapatna-562160, Karnataka, India.
Corresponding author: tngovi.phy@gmail.com

Abstract
The optical and thermal properties of binary mixtures of 4′-Octyloxy-4-biphenylcarbonitrile (8OCB) and 4-hexyl-4-biphenylcarbonitrile (6CB) materials under optical phase transition studies show that when the specimen cooled from its isotropic melt for the specified concentrations at different temperatures, respectively, re-entrant nematic and re-entrant smectic-A phases appeared sequentially. There has been discussion of electrical conductivity, activation energy, and charge carry mobility of re-entrant phases.
Keywords: *Optical studies: Electrical Conductivity: Re-entrant nematic and smectic phases: Activation energy: Charge mobility carriers:*

INTRODUCTION

In exploring the Liquid Crystals, miscibility is an essential parameter and verifying the types of mesophases. Calamitic systems made up of rod-like molecules frequently exhibit miscibility and Gibbs phase diagrams. As a result, eutectic blends with broad temperature working ranges for display materials have been created. Due to the temperature dependence of the nematic phase's thermal conductivity, the transport properties of nematic liquid crystals have been thoroughly investigated [1]. In order to improve the physical properties, expand the temperature range of liquid crystals, or decrease the melting point of liquid crystal phases, liquid crystal mixes are made. To lower the melting point of liquid crystal materials by creating eutectic mixtures and to expand the liquid crystal phase range for broader operating windows for display applications [2-4].

The present work shows that: different concentrations of 4′-Octyloxy-4-biphenylcarbonitrile (8OCB) and 4-hexyl-4-biphenylcarbonitrile (6CB) molecules indicate the presence of re-entrant nematic and re-entrant smectic-A phases at different temperatures.These phases have been documented by the use of the microscopic method.Electrical conductivity, activation energy, and transport properties of charge carrier mobility on different liquid crystalline phases have been discussed respectively at different temperatures.

EXPERIMENTAL SECTION

In the present study, we use the molecular compounds, namely: 4′-Octyloxy-4-biphenylcarbonitrile (8OCB) and 4-hexyl-4-biphenylcarbonitrile (6CB). Using benzene as a solvent it was subjected to purification twice by adopting the method of re- crystallization. For our experimental studies, we have considered the binary system of 8OCB molecules are at 65% of concentration and 35% concentration of 6CB molecules. To ensure homogeneity the ratio of given mixtures in desiccators is kept in exposures to many cycles of heating, stirring and centrifuging. Transition temperatures of given concentrations were measured using a Gippon-Japan polarizing microscope in conjunction with a hot stage. For microscopic observations the samples take their place on slide. Electrical-conductivity measurements of the mixture at differenttemperatures were carried out using digital LCR meter and a proportional temperature control unit [5-9].

International Journal of Environmental Sciences
ISSN: 2229-7359
Vol. 11 No. 20s, (2025)
https://theaspd.com/index.php/ijes

RESULTS AND DISCUSSIONS

LIQUID CRYSTALLINE PROPERTIES

The sample of binary mixture of Octyloxy and hexyl- biphenylcarbonitrile molecules, such as 65% concentrations of 8OCB and 35% concentrations of 6CB, displayed the molecular orientation of optical textures of re-entrant nematic and re-entrant smectic-A phases, as observed by the hot-stage Gippon-Japan-polarizing microscope. The concentrations of Octyloxy and hexyl- biphenylcarbonitrile group of molecules in this microscopic textural study show an extremely intriguing and unusual sequence of re-entrant nematic [10, 11] and focal conic domains of re-entrant SmA phases with an additional induced schileren texture of chiral smectic-C phases. These phases are obtained sequentially upon cooling the specimen from its isotropic phase. Microphotographs corresponding to the transitions of re-entrant nematic-re-entrant-smectic-A phases are observed under a microscope in Figure 1.

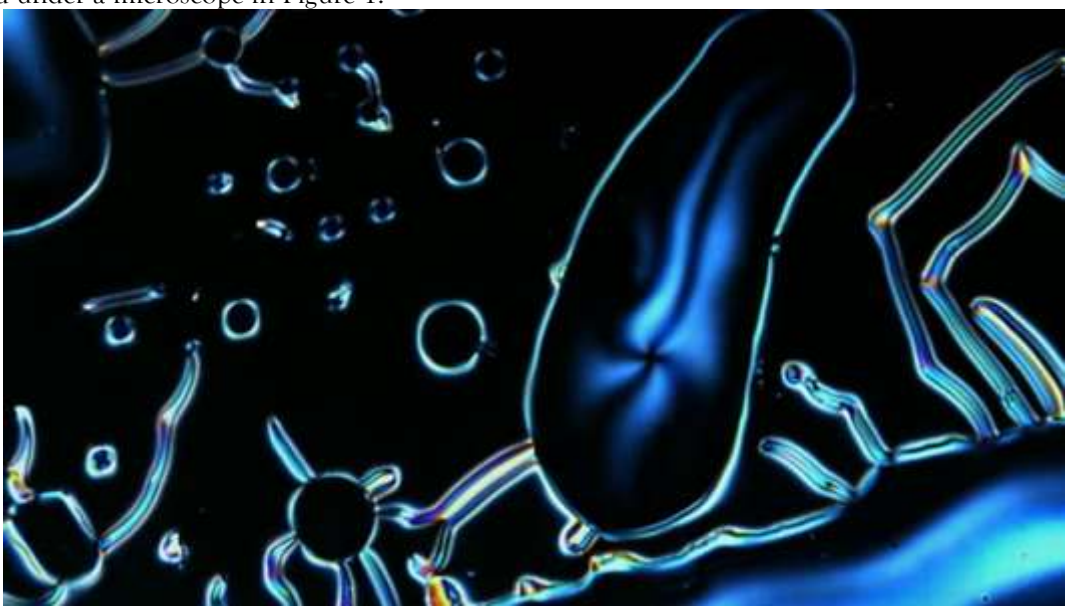

Figure 1: Microphotographs of Re-entrant nematic phase obtained between the crossed polars.

CONDUCTIVITY MEASUREMENTS

One of the main characteristics of liquid crystals that affect their technological uses is their electrical conductivity. A better understanding of the phase transition behavior with temperature can be gained through electrical conductivity studies. The lyotropic and thermotropic systems' phase behavior is related to a sudden rise or fall in electrical conductivity with temperature [12]. Figure 2 displays the temperature change of electrical conductivity for the 65% 8OCB in 6CB sample. Electrical conductivity reflects the shifts in molecular alignment and mobility when a liquid crystal transitions between phases; it is closely associated with phase behavior. Electrical-conductivity values were found to vary as we proceeded toward phase transitions from re-entrant nematic and re-entrant smectic-A phases, respectively. These changes corresponded to the optical-phase transition of liquid crystalline materials at different temperatures and were also used to identify the optical texture using a microscopic technique [13, 14]. A decrease in molecular alignment is indicated by an increase in conductivity, which leads to a freer moment of ions. The conductivity decreases as the molecular arrangement becomes more rigid. As the temperature drops, it has been found that the electrical conductivity continues to rise. This indicates the orientation order has a slight impact on the conductivity's magnitude. This implies that when the temperature drops, the size of the aggregated molecules increases and the system becomes more organized.

International Journal of Environmental Sciences
ISSN: 2229-7359
Vol. 11 No. 20s, (2025)
https://theaspd.com/index.php/ijes

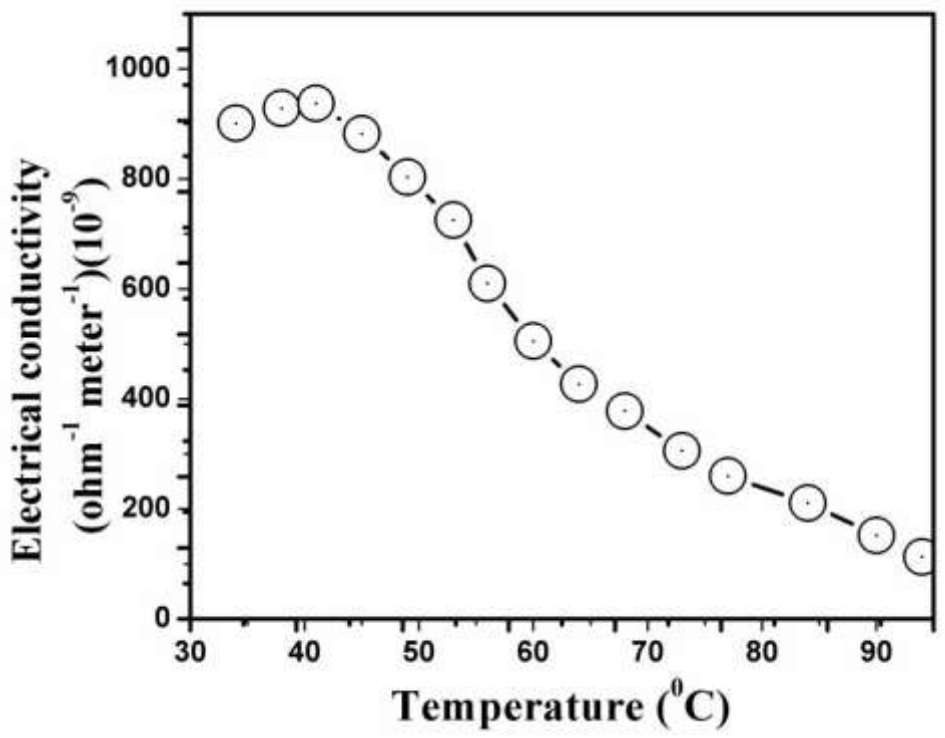

Figure 2.Temperature variation of electrical-conductivity for the sample 65% 8OCB in 6CB.

TEMPERATURE DEPENDENT ACTIVATION ENERGY ON RE-ENTRANT NEMATIC AND RE-ENTRANT SMECTIC PHASETRANSITION

Liquid crystals due to their unique phase between solid and liquid states, exhibit activation energy associate with molecular alignment and reorganization under external influences like temperature, electric fields or magnetic fields. The energy needed to overcome intermolecular forces that maintain the ordered structure of liquid crystal phase. Activation energy is often analyzed using the Arrehenius equation which relates variation of temperature with electrical conductivity.

$$\boldsymbol{\sigma = \sigma_o \, exp\left(E_a / K_B T\right)}$$

σ is the conductivity, σ_o is the pre exponential factor, E_a is the activation energy and K_B is the Boltzmann constant and T is the temperature. By using the conductivity data: Re arranging the given equation, once we can calculate the activation energy of liquid crystals phase transition between re-entrant nematic –re-entrant smectic-A is

$$\boldsymbol{E_a = K_B T \ln\left(\frac{\sigma}{\sigma_o}\right)}$$

The activation energy in the context of liquid crystal phase transition refers to energy required for the molecular re-organization necessary to transition from one liquid crystalline phase to another or to form an isotropic liquid phase. This energy barrier depends on molecular interactions, external conditions like temperature or electric fields and a specific liquid crystal structure.

Temperature variations of activation energy for the sample of 65% 8OCB in 6CB sampleis shown in figure 3. At a lower temperature region 30-45 ^{0}C, the graph shows steep rise in activation energy, which indicates that: the phase with more ordered molecular alignment such as the solid or crystalline phase. The increase in higher value of activation energy is the most suggestible higher potential barrier witnessed by the molecular dipole moment to orient at higher field. And it shows the surface activity of dispersed particles on local order of the liquid crystal; the increase in activation energy which lead to restrict the mobility of free charge carriers and hence it has low conductivity. Consequently the decrease in activation energy of the given molecules shows the existence of higher mobility of free charge carriers as it move towards crystalline phases with increase in conductivity of the order of nano meter. As increase in temperature, molecules are gain energy and henceit leads to increases the molecular movement and a transition to be less ordered state. The temperature region from 45-70^{0}C, the activation energy plateaus around 5-6 units and itsuggests transition in to liquid crystal state such as re-entrant nematic to re-entrant smectic-A phase. In these phases, the molecules have partial ordered-typical with directional alignment, but less positional ordered than a solid.At high temperature region greater than 70^{0}C, the graph levels off, it concluded that the activation energy stabilizes. These corresponds to the transition is a fully isotropic liquid phase, where the molecular order is completely lost. Here the liquid behaves like a conventional fluid with no directional alignment.The sharp increase in activation energy shows the solid to liquid crystal phase transition. The plateau corresponds to the liquid crystalline phase, characterized by a balance of order and disorder. The final leveling off of activation energy indicates liquid crystal to isotropic liquid transition [15-18].

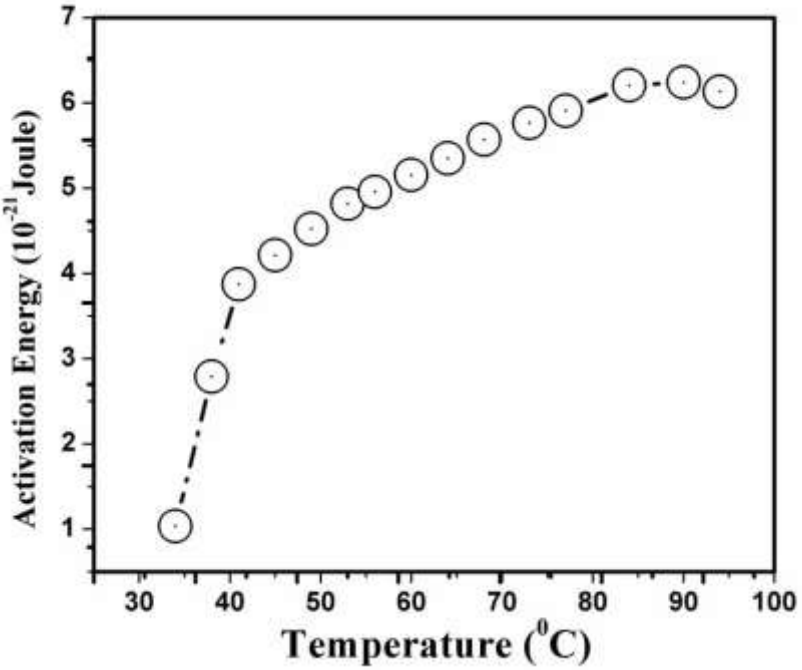

Figure 3.Temperature variations of activation energy for the sample of 65% 8OCB in 6CB.

International Journal of Environmental Sciences
ISSN: 2229-7359
Vol. 11 No. 20s, (2025)
https://theaspd.com/index.php/ijes

THE MOBILITY FREE CHARGE CARRIERS TRANSPORT ON RE-ENTRANT NEMATIC- RE-ENTRANT SMECTIC-A PHASES OF LIQUID CRYSTALS

Thermal activation causes mobility of free charge carriers to migrate between localized states, which are the main mechanism by which charge transport takes place in liquid crystals. The Pool-Frenkel or hopping transport models are frequently used to simulate the mobility of charge carriers are transport in disordered materials, such as liquid crystals. In such a system: The mobility of free charge carriers (μ) can be represented by the equation

$$\boldsymbol{\mu = \mu_o \exp\left(-\frac{E_a}{K_B T}\right) \exp\left(\beta \sqrt{E}\right)}$$

Where μ_o is the mobility at zero electric field, E_a is the activation energy for charge hopping, K_B is the Boltzmann constant, T is the temperature, E is the electric field and β is a field dependent constant that reflects the influence of the electric field on the mobility.

This equation illustrates how the mobility of free charge carriers is affected by both thermally activated energy and a constant electric field at varying temperatures and between isotropic and crystalline phases. Figure 4 below illustrates how free charge carrier mobility changes with temperature in a constant electric field.

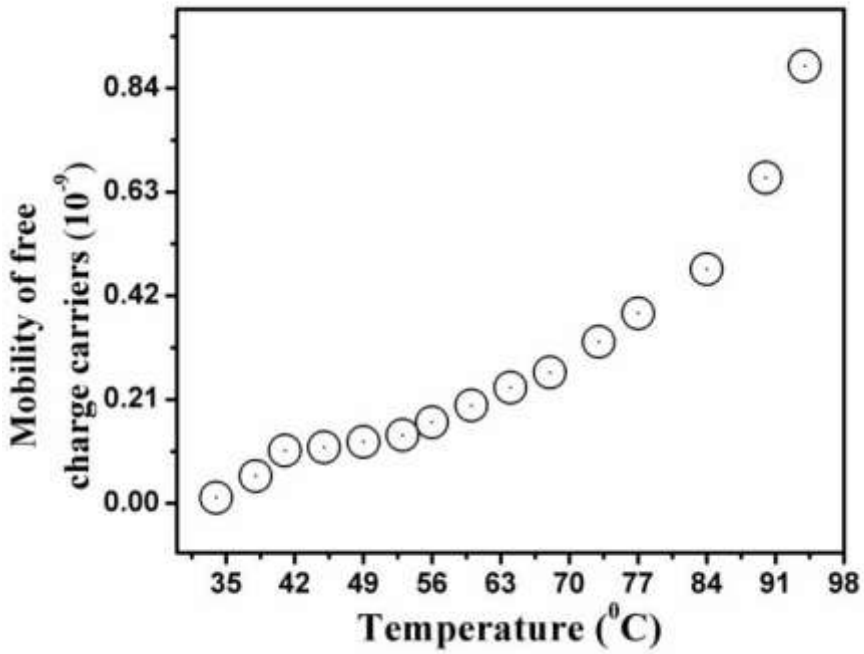

Figure 4 shows how temperature variations affect the movement of free charge carriers. The liquid crystalline phases in the current study have very little mobility with a constant electric field of 5 volts. Free charge carrier mobility and temperature during a phase transition from a re-entrant nematic phase to a re-entrant smectic-A phase are depicted in the graph. In the low temperature range of 35 to 70^{0}C, free charge carrier mobility is comparatively modest and increases gradually as temperature rises. The molecular configuration permits a reasonable degree of mobility for the movement of charge carriers, which is consistent with the re-entrant nematic phase. Mobility increases dramatically with temperature as the temperature rises from 70 to 84^{0}C. The change from the re-entrant nematic to the re-entrant smectic-A phase is shown by this. As the system starts to rearrange its molecular structure, the thermal energy increases the mobility of the charge carriers. The mobility

saturates or grows less dramatically when the temperature rises between 84 and 98 ^{0}C. The molecules create layered structures in the re-entrant smectic-A phase, which is represented by this. Stabilization mobility values result from these layers' restriction of charge carriers' free motion. Charge carriers can travel more easily in the nematic phase because molecules are more disorganized there. A thermal agitation aids in a minor improvement in mobility as the temperature rises. The system organizes into layers during the shift to the smectic-A phase, and this restructuring affects the flow of charge carriers. Increased thermal energy causes mobility to rise initially, but the structured environment eventually restricts further mobility growth. The intricate relationship between molecular organization and thermal energy during the phase transition is thus depicted in the graph. Advanced LCD technologies with enhanced electro-optical properties, thermal stability, and response characteristics can be developed by scientists and engineers by examining the mobility of charge carriers between re-entrant nematic and smectic-A phases [19-21].

CONCLUSIONS

Optical microscopic analysis of the binary combination of 4-hexyl-4-biphenylcarbonitrile (6CB) and 4′-Octyloxy-4-biphenylcarbonitrile (8OCB) at varying temperatures clearly highlight the presence of re-entrant nematic to re-entrant smectic-A for the specified concentrations. The threshold voltage and switching speeds of liquid crystal displays are directly impacted by changes in charge carrier mobility. Devices that use re-entrant liquid crystals exhibit different contrast levels and response times depending on the phases. Scientists and engineers can create cutting-edge LCD technologies with enhanced electro-optical qualities, thermal stability, and response characteristics by researching the mobility of charge carriers across re-entrant nematic and smectic-A phases of liquid crystals.

REFERENCES

[1] P. G. de Gennes, The Physics of Liquid Crystals, 2nd ed. (Oxford University Press, Oxford, 1993.
[2] Satyendrakumar. Liquid crystals: Experimental study of physical properties and phase transitions).Cambridge University Press. 2001.
[3] Oleg D. Lavrentovich. Defects in Liquid Crystals: Computer Simulations:Theory and Experiments. 2002.
[4] P J Coolings and J W Goodby. Introduction to Liquid Crystals Chemistry and Physics.2nd Edtn: 2020. Taylor & Francis Group, LLC.
[5] Nagappa, S. K. Nataraju, and D. Krishnamurthy. Mol. Cryst. Liq. Cryst.133.31. 1986.
[6] T. N.Govindaiah Mol. Cryst. Liq. Cryst. 626 (1).141-150. 2016.
[7] J. Theim,V. Vill and F. Fischer. Mol. Cryst. Liq. Cryst. 170:43. 1989.
[8] A. Lovely Jacob and Babu, J.Res. Scholar. II.143. 2012.
[9] T. N.Govindaiah. Mol. Cryst. Liq. Cryst. 624 (1).20-27. 2016.
[10] W. S. Braga, N. M. Kimura, D. D. Luders, A. R. Sampaio, P. A. Santoro and A. J.Palangana. The European Physical Journal E. . 24. 247-250. 2007.
[11] T. N. Govindaiah. Mol. Cryst. Liq. Cryst. 625 (1). 93-98. 2016.
[12] M. Marthandappa, Nagappa, K. M. LokhanathaRai, J. Phys. Chem.95(16). 6369-6372. 1991.
[13] T. N. Govindaiah, H. R. Sreepad, Nagappa, Mol.Cryst. Liq. Cryst..593. 51-60. 2014.
[14] T. N. Govindaiah, H. R. Sreepad, Nagappa, Mol. Cryst. Liq.Cryst.592. 82-90. 2014.
[15] Shuguang Li, Kodi Raghunath, Ayman Alfaleh, Farhan Ali, A. Zaib, M. Ijaz Khan, Sayed M. ElDin and V.Puneeth. www.nature.com/scientificreport.13.2666. 2023.
[16] T.N. Govindaiah Mol.Cryst. Liq. Cryst.,625 (1). 99-105. 2016.
[17] F. Wang.et al. Nanotechnol. Rev. 11.1620-1632. 2022.
[18] Mahes and Prajapti. J. Phy. Che of Sol.71(12).1684-1689. 2010.
[19] G. Derfel and A. Lipiński. Mol.Cryst. Liq. Cryst.55. 89-100. 2011.
[20] Jun-ichi Hanna, Akira Ohno, Hiroaki Iino. Thin Solid Films. 554.58-63.2014.
[21] T.N. Govindaiah. Mol.Cryst. Liq. Cryst. 626 (1). 151-159. 2016 .