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Research on Various Display Properties of a Room-Temperature Twisted Nematic Display Material 6CHBT by Doping Single-Walled Carbon Nanotubes

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KEYWORDS

SWCNTs, Nematic Displays, 6CHBT, ^{1}H-NMR, ^{13}C-NMR, Dielectric Permittivity, Loss, Relaxation Frequency, Dielectric Anisotropy, and Display Parameters.

ABSTRACT:

Present studies concentrate on the optical, dielectric, and electro-optical properties of single-walled carbon nanotubes (SWCNTs) doped in the nematic matrix of the liquid crystalline material 4-(trans-4′-*n*-hexylcyclohexyl)isothiocyanatobenzene (6CHBT). 6CHBT is the nematic liquid crystalline substance that was employed in the investigation. SWCNTs having a diameter of around 0.8-1.4 nm and a length of about 100-300 nm have been inserted into it. For displays, the nematic liquid crystalline material 6CHBT is a perfect basis material due to its nematic phase temperature range of 12.5 - 43.0 °C. SWCNTs have been doped in 6CHBT in two different concentrations i.e., 0.01 and 0.02% (weight ratio). For higher concentrations, CNTs were observed to be bundled at different locations. For this reason, higher concentrations were not studied. Using electro-optical and dielectric spectroscopy, the effects of SWCNTs doping on a number of display characteristics, including threshold voltage, dielectric anisotropy, and splay elastic constant, have been investigated. SWCNTs alignment parallel to the nematic direction is supported by the nematic phase. Nevertheless, in the nematic phase, the SWCNTs improve the molecules' local orientational arrangement. Consequently, the use of SWCNTs considerably reduces the threshold voltage required to change the geometry of the molecules from planar (bright state) to homeotropic (dark state).

1. Introduction

Since nanoparticles and nanotubes have extraordinary electrical, optical, and magnetic capabilities, researchers have become more and more interested in them[1]. Nanoparticles have been effectively used in some studies to enhance the electro-optical properties of materials used in liquid crystal displays[2–8]. The majority of the time, nanoparticles lowered the threshold voltage (V_{th}) required to cause the molecules to shift from a planar to a homeotropic form. Electron beam irradiation (EBI) was used to enhance the electro-optical (E-O) properties of 5CB, a nematic liquid crystal display material[9]. The dielectric anisotropy of the material may be modified to improve the steepness of the transmission-voltage (T-V) curve by employing an appropriate dose of electron beam irradiation; however an increase in the threshold voltage was seen. In the present study, we demonstrate that the display properties (threshold voltage, dielectric anisotropy, and splay elastic constant) of another room-temperature nematic liquid crystalline material were altered by the doping of single-wall carbon nanotubes (SWCNTs). The substance employed in the investigation is 4-(trans-4'-*n*-hexylcyclohexyl)isothiocyanatobenzene (6CHBT), a nematic liquid crystal. SWCNTs with a diameter of

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0.8 to 1.4 nm and a length of 100 to 300 nm have been added to it. The nematic liquid crystalline substance 6CHBT, which has a temperature range of 12.5–43.0 °C and low viscosity, makes it an ideal base material for displays[10]. Readers interested in learning more about the electrical and electro-optical characteristics of a room-temperature twisted nematic display material 6CHBT by doping single-walled carbon nanotubes can read our previously published research work[11].

2. Experimental Techniques

To manufacture the cells with electrode spacing (d) of 5 μm, polymer-coated and parallel-rubbed Indium tin oxide (ITO)-coated glass plates with a pre-tilt angle of 1-3° were employed. From Instec in the USA, these cells were bought. In these cells, molecules are arranged parallel to the direction that the glass plates rub against one another. The static value of the transverse component of relative dielectric permittivity ($\varepsilon_{\perp}'$) was calculated using the same cell. Nevertheless, to produce the cells for the measurement of the longitudinal component of relative dielectric permittivity ($\varepsilon_{||}'$), gold coated glass plates with an additional coating of lecithin were utilized. Using a polarized light microscope and a photo-detector device from Instec, E-O characteristics (T-V curves) were created. Using a six and a half digit multimeter, the photo-voltage (which is proportional to the intensity of the transmitted light) obtained from the photo-detector was recorded. The T-V data was used to calculate V_{th}. Using an impedance meter (N4L, model PSM-1735) linked with an impedance analyzer interface, dielectric permittivity measurements were collected in the frequency range of 1 Hz to 35 MHz in order to identify further display characteristics. A hot stage with an accuracy of ± 0.1°C (Instec, model HS-1) was used to regulate the sample's temperature. As there are no low- or high-frequency artifacts[12-14] and no dispersion mechanism up to this frequency, the 10 kHz dielectric measurements have been regarded as the "static" values. The relative dielectric permittivity $\Delta\varepsilon'$ ($= \varepsilon_{||}' - \varepsilon_{\perp}'$) anisotropy has been determined using this data. Additional details about the experimental setup and procedures used to get the dielectric measurements are available in previous publications[14, 15].

3. Results and discussion

SWCNTs have been doped in 6CHBT in two different concentrations, i.e., by weight ratio: 0.01 and 0.02%. Figure 1 shows an optical texture that validates a homogenous distribution of SWCNTs up to 0.02% in the nematic matrix of 6CHBT. The bright areas in Figure 1 are caused by the erroneous homeotropic orientations of the 6CHBT molecules with respect to the SWCNTs. Nevertheless, it was demonstrated that CNTs were bunched in different locations for greater concentrations. For this reason, higher amounts were not investigated. Table 1 displays the T-V data for both pure and SWCNT-doped 6CHBT samples at 22.0 °C. A brilliant state occurs when molecules are oriented planarly at low voltages ($<V_{th}$). When the applied voltage rises over V_{th}, molecules eventually adopt a homeotropic orientation (molecular director normal to the electrode surface), and dark condition is observed. Switching voltage interval is the voltage needed to shift the intensity from 90% of the maximum value to 10%. The switch voltage interval serves as a gauge for the T-V curve's steepness. The threshold voltages that were obtained using these T-V values are listed in Table 2.

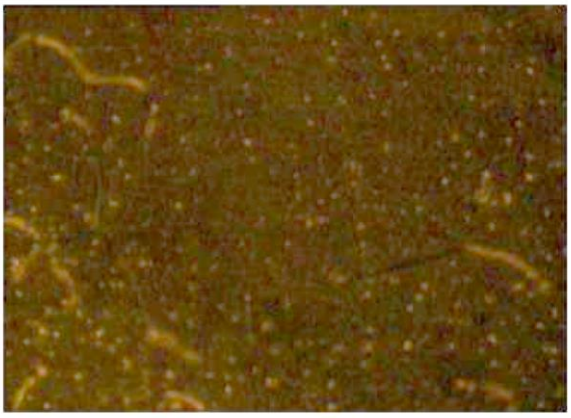

Figure 1: The optical texture of 6CHBT doped with 0.02% SWCNT is presented under homeotropic circumstances. The propagation of SWCNTs is depicted by bright spots on a dark field of view (caused by the 6CHBT molecules surrounding the nanotubes orienting incorrectly homeotropically).

Journal of Chemical Health Risks

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JCHR (2023) 13(4s), 829-834 | ISSN:2251-6727

Table 1: T-V values are for both pure 6CHBT and SWCNTs-doped 6CHBT samples at 22.0 °C.

Pure 6CHBT System		**Dispersed System**			
		6CHBT + 0.01% weight ratio SWCNTs		**6CHBT + 0.02% weight ratio SWCNTs**	
Applied Voltage (Volts)	**Photo Voltage (Volts)**	**Applied Voltage (Volts)**	**Photo Voltage (Volts)**	**Applied Voltage (Volts)**	**Photo Voltage (Volts)**
0.10	6.00	0.10	5.90	0.10	5.80
0.30	6.00	0.30	5.90	0.30	5.80
0.70	6.00	0.50	5.90	0.50	5.80
0.80	6.00	0.70	5.90	0.70	5.80
0.90	6.00	0.90	5.90	1.10	5.80
1.10	6.00	1.10	5.90	1.40	5.80
1.30	6.00	1.30	5.90	1.60	5.80
1.50	6.00	1.50	5.90	1.90	5.80
1.70	6.00	1.70	5.90	2.10	5.80
1.90	6.00	1.80	5.90	2.10	5.80
2.10	6.00	1.90	5.90	2.30	5.80
2.20	6.00	2.00	5.90	2.50	5.80
2.30	6.00	2.10	5.90	2.80	5.80
2.50	6.00	2.20	5.90	3.00	5.80
2.70	6.00	2.30	5.90	3.10	5.80
2.80	6.00	2.40	5.90	3.20	5.80
2.90	6.00	2.50	5.90	3.50	5.80
3.10	6.00	2.70	5.90	3.70	5.80
3.20	6.00	2.90	5.90	3.90	5.80
3.30	6.00	3.10	5.90	4.10	5.80
3.40	6.00	3.30	5.90	**4.40**	5.80 ↓
3.50	6.00	3.50	5.90	4.90	4.68
3.60	6.00	3.70	5.90	5.30	3.36
3.70	6.00	3.90	5.90	5.70	2.08
3.80	6.00	4.10	5.90	6.20	1.12
3.90	6.00	4.30	5.90	6.70	0.20
4.10	6.00	4.50	5.90	7.00	0.00
4.20	6.00	4.70	5.90	7.40	0.00
4.40	6.00	**4.90**	5.90 ↓	7.60	0.00
4.80	6.00	5.10	5.12	7.90	0.00
5.00	6.00	5.50	4.04	8.20	0.00
5.20	6.00	5.70	3.16	9.00	0.00
5.50	6.00 ↓	5.80	2.08	9.20	0.00
5.70	5.84	6.10	1.44	10.10	0.00
6.20	3.64	6.30	1.04	10.60	0.00
6.50	2.40	6.50	0.60	11.10	0.00
7.00	1.56	6.70	0.28	11.30	0.00
7.40	1.24	7.00	0.00	11.60	0.00
7.70	1.00	7.20	0.00	11.90	0.00
8.10	0.36	7.40	0.00	12.30	0.00
8.60	0.00	7.70	0.00	12.50	0.00
9.20	0.00	8.10	0.00	12.70	0.00
9.50	0.00	8.60	0.00	13.30	0.00

Journal of Chemical Health Risks
www.jchr.org
JCHR (2023) 13(4s), 829-834 | ISSN:2251-6727

11.10	0.00	8.90	0.00	13.80	0.00
11.80	0.00	9.20	0.00	14.30	0.00

Table 2: The threshold voltage (V_{th} with DC field and at 22.0 °C), and relaxation frequency (f_r) corresponding to flip-flop motion of molecules about their short axes at 22.0 °C.

Sample → / Various Parameters ↓	**Pure 6CHBT System**	**6CHBT + 0.01% weight ratio SWCNTs**	**6CHBT + 0.02% weight ratio SWCNTs**
V_{th} (volts)	5.5	4.9	4.4
f_r (MHz)	1.47	1.68	2.93
K_{11} (N)	1.40×10^{-10}	1.37×10^{-10}	1.24×10^{-10}
τ_{off} (ms)	250	280	350

Table 3: The pure 6CHBT and SWCNTs-doped 6CHBT system's electrical parameters at 22.0 °C.

Pure 6CHBT System at 22.0 °C	
Electrical Parameters	**Values**
$\varepsilon'_{\parallel}$	10.90
$\varepsilon'_{\perp}$	5.70
$\Delta\varepsilon'$	5.20
$\Delta\varepsilon'/\varepsilon'_{\perp}$	0.91
6CHBT + 0.01% weight ratio SWCNTs at 22.0 °C	
Electrical Parameters	**Values**
$\varepsilon'_{\parallel}$	11.48
$\varepsilon'_{\perp}$	5.22
$\Delta\varepsilon'$	6.26
$\Delta\varepsilon'/\varepsilon'_{\perp}$	1.19
6CHBT + 0.02% weight ratio SWCNTs at 22.0 °C	
Electrical Parameters	**Values**
$\varepsilon'_{\parallel}$	11.96
$\varepsilon'_{\perp}$	5.01
$\Delta\varepsilon'$	6.95
$\Delta\varepsilon'/\varepsilon'_{\perp}$	1.38

Table 4: The least-squares regression line equations and correlation coefficient (R^2) for pure and doped systems using the slopes of straight lines.

Sample	**Least-Squares Regression Line Equations**	**Correlation Coefficient (R^2)**
Pure 6CHBT System	Log (f_r) = -3.4178 (1000/T) + 17.745	0.9557
6CHBT + 0.01% weight ratio SWCNTs	Log (f_r) = -3.4714 (1000/T) + 17.959	0.9656

Journal of Chemical Health Risks

www.jchr.org

JCHR (2023) 13(4s), 829-834 | ISSN:2251-6727

6CHBT + 0.02% weight ratio SWCNTs	Log (f_r) = -2.9571 (1000/T) + 16.475	0.9659

It is evident from Table 1 and Table 2 that as SWCNTs doping concentration is increased, V_{th} greatly reduces, which is advantageous from an application standpoint. Due to the doping of SWCNTs, the T-V curve's steepness is also becoming better. Table 3 shows that the concentration of SWCNTs causes $\Delta\varepsilon'$ to increase. The computed splay elastic constant, K_{11}, based on the experimental data for V_{th} and $\Delta\varepsilon'$ are displayed in Table 2. Table 2 demonstrates that while SWCNTs doping concentration raises, V_{th} and K_{11} decrease. The time required for homeotropic to planar switching (τ_{off}), as determined by the measurement of the optical response (under square pulse), increases with SWCNTs doping; for pure 6CHBT, this time is 250 ms, while for 0.01 and 0.02% SWCNTs doped in 6CHBT, it is 280 and 350 ms, respectively as mentioned in Table 2. τ_{off} is inversely proportional to K_{11} ($\tau_{off} = \gamma d^2/\pi\ K_{11}$ with γ being rotational viscosity of the material) and therefore increase of τ_{off} also supports decrease of K_{11} due to the presence of SWCNTs in 6CHBT.

The degree to which two variables are linearly related, or change together at a constant rate, is expressed statistically by correlation. It's a popular method for summarizing straightforward relationships without establishing causation and effect. The movement of one variable in relation to another is described by the correlation coefficient (R^2). A score of 1 indicates a perfect positive correlation, meaning that the two move in the same direction when there is a positive correlation.

The smallest quantity of energy required for reactants to be accessible in order for a chemical reaction to take place is known as activation energy in the Arrhenius model of reaction rates. Kilojoules per mole (kJ/mol) or kilocalories per mole (kcal/mol) are units of measurement for activation energy (E_a) of a process. Activation energy is the least additional energy needed by a reacting molecule to transform into a product. The bare minimum of energy required energizing or activating molecules or atoms in order for them to go through a chemical reaction or transformation is another way to put it.

Relaxation frequencies follow Arrhenius equation[17]: $f_r = A \exp(-E_a/N_A kT)$. Where E_a is the activation energy associated to the flip-flop motion of molecules along their short axes, N_A is the Avagadro number, and k is the Boltzman constant.

The brief lag in a material's dielectric constant is known as dielectric relaxation. This is typically brought on by the molecular polarization delay in a dielectric medium (such as between two large conducting surfaces or inside capacitors) in response to a varying electric field. The relaxation frequency (f_r) is the frequency at which the dielectric loss factor (ε'') reaches a maximum, for a dielectric material that has no static (d.c.) conductivity and that is subjected to an alternating electric field.

A type of mathematical regression analysis called least squares is used to find a set of data's line of best fit, which shows the relationship between the data points visually. The least-squares regression line equation is y = mx + b, where m is the slope. The least-squares regression line equations for pure and doped systems using the slopes of straight lines are shown in Table 4.

The method of least square fit has been used to determine the slopes of the log (f_r) vs. inverse of temperature plots. Using the slopes of straight lines, almost equal activation energies (63±2 kJ/mole) for pure and doped systems have been found.

4. Conclusions

The experimental results for pure, with 0.01% and 0.02% SWCNTs in 6CHBT, are summed up as follows:

1. The liquid crystalline material 4-(trans-4′-*n*-hexylcyclohexy)isothiocyanatobenzene (6CHBT) have been synthesized at laboratory through standard operating procedure. It was separated out, dried and melting point was recorded on Toshniwal Electronic Melting Point Apparatus. Analysis was confirmed by calculating C, H, N, S via mass % of the sample. The ^{1}H NMR and ^{13}C NMR were recorded which confirms that the compound was successfully synthesized.
2. The variations of longitudinal ($\varepsilon_{||}'$) and transverse ($\varepsilon_{\perp}'$) components of relative permittivity with temperature (°C) and hence dielectric anisotropy ($\Delta\varepsilon' = \varepsilon_{||}' - \varepsilon_{\perp}'$) with temperature increases due to the presence of SWCNTs in the nematic matrix of 6CHBT.
3. All of the examined samples, which are pure and contain 0.01% and 0.02% SWCNTs in 6CHBT, have positive dielectric anisotropy.
4. It has been demonstrated that the splay elastic constant decreases with the addition of SWCNTs to the nematic matrix of 6CHBT.

Journal of Chemical Health Risks

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5. Thus, these two properties lead to a considerable reduction in the threshold voltage required to convert a molecule's conformation from planar (bright state) to homeotropic (dark state).
6. The nematic matrix supports the orientation of the SWCNTs parallel to the nematic direction. Conversely, the local orientational ordering of molecules in the nematic phase is enhanced by the presence of SWCNTs, most likely due to strong van der Waals contacts and a concomitant increase in the nematic order parameter.
7. When molecules flip-flop about their short axes, the relaxation frequency that corresponds to that motion increases. Relaxation frequency increases as SWCNTs doping concentration increases. The useful frequency range for display applications, which is below the relaxation frequency, increases as the doping concentration increases.

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