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Photo tuning of thiophene-2, 5-dicarbohydrazide derivatives for their photoalignment ability-Molecular modelling studies

Gurumurthy Hegde ^a*, A. A. Murausky,^b A. A. Murauski,^b I. N. Kukhta,^b A. V.

Adhikari,^c L.Komitov,^d

In this work, we reported a photoalignment of a nematic liquid crystal, promoted by thin alignment layers made from novel thiophene-2,5-dicarbohydrazide derivatives after being illuminated with linear polarized UV light. A clear indication about the relationship between molecular structure and alignment properties of the materials were obtained by introducing a methyl substituent group (-CH₃) in the molecular structure of some of the materials studied in this work. Interestingly, the illumination with linear polarized UV caused the preferred direction of liquid crystal alignment, promoted by these layers, to be oriented either parallel (in case of thiophene derivative without methyl substitution) or perpendicular (in case of thiophene derivative with methyl substitution). Mechanism behind the observed alignment effect is elucidated by molecular modelling studies. These studies suggested the change of the orientation of the materials, as a possible origin. Such information is indispensable for the design and synthesis of novel photo-alignment materials for liquid crystal displays of high quality.

1. Introduction

The alignment quality of the liquid crystal in liquid crystal displays (LCD) is of vital importance for the performance of these devices. The conventional alignment technique used at present in the fabrication of LCDs is the mechanical rubbing of the alignment layers deposited onto the inner surface of the supporting glass substrates. This alignment technique, however, generate mechanical defects and electrostatic charges which may damage the TFT elements in LCDs as well as the optical appearance of the device, deteriorating the performance of LCDs.

Another alignment technique, attracted recently a lot of interest from the LCD industry, is the photoalignment (PhA). This alignment method is a non-contact method and therefore it does not generate any electrostatic charges or mechanical defects which is a big advantage compared to the rubbing alignment method.

PhA method is based on new materials and techniques. Although in a very limited scale, this alignment method is already employed in the LCD industry [1–6]. Many materials capable to align liquid crystals (LC) have been discovered lately and used for preparation of alignment layers in LCDs [7, 8]. However, the lack of proper materials for photoalignment layers in LCDs is still a serious obstacle for application of this technique in the LCD industry in a broader scale. There are a number of requirements to the conventional materials used for preparation of alignment layers in LCDs such as long term chemical, physical and electro-chemical stability as well as high voltage holding ratio (VHR), low residual dc (RDC) and proper anchoring properties (low or strong anchoring strength, depending on the particular LCD application). In addition to these requirements, the materials for photoalignment layers in LCDs need to be highly photosensitive so that light with low light intensity and short exposure time will give sufficiently large photoalignment effect, which is stable with time and ambient illumination.

Generally, there are two groups of materials for photoalignment layers. One group consist of materials, which promote planar alignment (PA) of the liquid crystal molecules due to directional photo-degradation of the alignment layer exposed to illumination with linearly polarized UV light. The other group of photoalignment materials exhibit a photoalignment effect due to photochemical reaction, such as photoisomerization, photodimerization, photodirected crosslinking, etc., which take place in these materials under illumination with linearly polarized UV light [7].

Photoalignment effect may give preferred orientation of the liquid crystal molecules parallel or perpendicular to the polarization plane of UV light [9, 10] depending [9, 10] on the molecular structure of the material. Molecular structure is also of vital importance for the magnitude of anchoring energy of the promoted PhA, which has

very strong impact on the LCD performance. Therefore, the knowledge of the relations between the molecular structure of the materials for photoalignment layers and LCD characteristics is of vital importance for achievement of the desired performance of LCDs.

Thiophene derivatives have been investigated as liquid crystalline materials [11] but very little work has been reported on their application as photoalignment materials in LCD. The inherent properties and structure of thiophene moiety, synthesis and liquid crystalline properties of thiophene derivatives have been extensively investigated and the results are reported in [12, 13]. The most interesting feature is that the introduction of thiophene, a five membered heterocycle, develops a kink or bend in the molecule structure as an electrophilic substitution can be achieved at apositions (C-2 and C-5) in preference to the β -positions (C-3 and C-4) there by producing nonlinear geometry in the molecule. An exocyclic bond angle of 147.5° can be obtained by 2,5-disubstitution giving rise to a kink or bend in the molecular structure. Hence, incorporation of suitably substituted thiophene tends to lower both the melting point and the clearing point in comparison with the classical design of liquid crystals, based on 1,4-phenylene rings (exocyclic bond angle, 180°) in the molecular core [12] and the presence of a highly polarisable electronegative sulfur atom imparts a transverse dipole moment, avoiding the need for additional lateral substituents. Seed [12] has mentioned liquid crystalline character of some 2,5-disubstituted thiophenes in his review of thermotropic liquid crystals derived from thiophene and related five-membered heterocycles. On the other hand, certain 2,5-thienylene derivatives are structurally planar and electrically conductive making them useful in electronic applications. Liquid crystalline properties of esters derived from chiral 2-octanol and comprising 2,5-disubstituted thiophene have been reported [13, 14]. In certain cases, 2,5disubstituted thiophene-based chiral esters exhibited SmC* ferroelectric, ferrielectric and antiferroelectric phase sequence, suggesting application in electro-optical devices [13, 14].

Recently, we reported study on fluorine based derivatives of 1,3,4oxadiazole where changes in the molecular structure of this compound, such as incorporation of mono fluoro and difluroro substituents, bring the molecules to parallel and perpendicular orientation, respectively, with respect to the polarization plane of the UV illumination [15]. We applied this very simple idea of changing the alignment of the liquid crystal promoted by alignment layer made from thiophene derivatives by means of insertion of functional groups in their molecular structure. In light of this herein we explored the PhA properties of differently substituted thiophene composed bis hydrazones. Depending on their structure these compounds promoted either parallel or perpendicular alignment of the liquid crystal with respect to the polarization plane of UV illumination. The molecular modeling study has been conducted to explain their photoalignment behavior.

In this work we report the results of our study on the impact of the molecular structure of several thiophene composed bis hydrazones on the alignment properties of layers made from these materials.

2. Experimental details

2.1. Materials and Instrumentation

All chemicals were purchased from Aldrich and used without further purification. Melting points were determined by open capillary method and were uncorrected. Elemental analysis was performed on Thermo Fin ningan FLASHEA 1112CHN analyser. IR spectra (KBr pellets) were recorded on a Shimadzu FT-IR 157 spectrophotometer. ¹H-NMR spectra were recorded on a BRUKER AMX 400MHz spectrometer using TMS as internal standard. Mass spectra were recorded on LCMS-Agilent 1200 series with MSD using 0.1% aqueous TFA in acetonitrile system on C18-BDS column for 10 min duration. Ionization mode is E1 for all the compounds. The purity of the compounds was checked by TLC silica coated plates obtained from Merck.

Four different thiophene derivatives, assigned as T1-T4, with structure depicted in the supplementary file were studied here. Each of thiophene derivatives, were dissolved separately in THF solvent with concentration of 1 wt%. With these solutions, photoalignment layers were prepared according to the following procedures. The solution was spin coated onto the surface of previously cleaned glass substrates for 10sec at 800rpm followed by 20sec at 2000 rpm. After that the substrates were heated for 15min at 100°C, which resulted in thin films of the thiophene derivatives on the glass substrates' surface with thickness of about 50nm. The substrates covered with photoresponsive thiophene films were exposed to linearly polarized UV light using standard USHIO light exposure system equipped with deep medium pressure mercury lamp giving 3mW/cm² linearly polarized UV light passing through polarizer and light filter cutting the light below 290nm. After UV light illumination, conventional liquid crystal sandwich cells were prepared with these glass substrates with a cell gap of 3-4µm. Nematic liquid crystal MLC $6873 - 100 (\Delta \epsilon > 0)$ was filled in the isotropic phase in the cell gap via capillary forces. The quality of PhA in the cells, promoted of each of the thiophene derivatives, was determined by polarizing optical microscope with crossed polarisers. The direction of the preferred liquid crystal alignment, promoted by the thiophene PhA layer, was defined by means of λ first-order red plate [16].

2.1. Molecular modelling studies

The theoretical calculations for thiophene derivatives T_1 - T_4 have been carried out using the Gaussian 03 quantum chemical package [17]. The computations have been performed using the density functional theory (DFT) with the popular hybrid B3LYP functional at the basis set level of 6–31G. The gas phase ground state molecular geometries were fully optimized without imposing any molecular symmetry constraints. Next the general molecular dipole moments and the intramolecular distribution of transverse and longitudinal dipole moments localized on the side groups were computed and analyzed.

2.2. Synthesis

Synthesis of 3,4-di(substituted)thiophene-2,5-carbonyldihydrazide

Exactly 0.003 mole of diethyl 3,4-propyloxythiophene-2,5dicarboxylate was added to a solution of 0.03mol of hydrazine hydrate in 30mL of absolute ethanol. The reaction mixture was refluxed for 2 h. Upon cooling the reaction mixture, white precipitate was obtained. The product was then filtered, washed with alcohol and dried to get required compounds with good yield. The compound was crystallized using ethanol/chloroform.

¹H NMR (400 MHz, CDCl₃), d (ppm): 1.03 (t, 6H, -CH₃, J = 7.4 Hz), 1.76–1.85 (m, 4H, >CH₂), 4.11 (t, 4H, -OCH₂-, J = 6.8 Hz),

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4.98 (s, 4H, -NH₂), 8.34 (s, 2H, >NH). FTIR (KBr, cm⁻¹): 3338, 3290(>N-H), 3195, 2966, 2931, 2875, 1656 (>C=O), 1503, 1375, 1306, 1062, 949, 637. Elemental analysis data's for $C_{12}H_{20}N_4O_4S$: C, 45.56; H, 6.37; N, 7.71; S, 10.14. Found: C, 45.46; H, 6.41; N, 7.69; S, 10.05.

General procedure for synthesis of bis-hydrazides (T₁-T₄)

A clear solution of 0.005 mole of 3, 4-disubstituted thiophene carbohydrazide in 15 mL of absolute ethanol was mixed with 0.5 mL of cone. hydrochloric acid. To this 0.01 mole of appropriate carbonyl compound, dissolved in 10 mL of absolute ethanol was added slowly while stirring. The reaction mixture was heated to reflux for 4 h and cooled to 10° C. The precipitated product was separated by filtration and re-crystallized from an appropriate solvent. The physical and characterization data of all newly synthesized compounds are presented in Table 4.1. Spectral data of some of the compounds are given below along with their re-crystallization solvent.

3,4-Dipropoxy- N^2 , N^5 -bis(thiophen-2-ylmethylene)thiophene-2,5-dicarbohydrazide (T₁)

M.P: 259-260 °C. FTIR (KBr, cm⁻¹) v: 3222 (-NH-), 2966 (propyl), 1641 (>C=O) and 1592 (>C=N-); ¹H NMR (DMSO-d₆, 400 MHz) δ in ppm: 0.9 (t, 6H, -CH₃, J=6.9Hz), 1.7 (m, 4H, -CH₂-,), 4.2 (t, 4H, -OCH₂- J=6.7 Hz), 7.1 (t, 2H, C₄-thiophene), 7.4 (d, 2H, C₅-thiophene) and 7.6 (d, 2H, C₃-thiophene, J=4Hz), 8.6 (s, 2H, -N=CH-), 11.2 (s, 2H, -CONH-); MS (m/z, %): 504 (M⁺, 100), 378 (50), 352 (20), 294 (40), 227 (20), 169 (30), 154 (40). Elemental analysis; C₂₂H₂₄N₄O₄S₃: Estimated C, 52.36%; H, 4.79%; N, 11.10%; S, 19.06%. Found: C, 52.30 %; H, 4.68 %; N, 11.32%; S, 19.11%.

3,4-dipropoxy- N^2 , N^5 -bis(1-(thiophen-2-yl)ethylidene)thiophene-2,5-dicarbo hydrazide (T₂)

M.P:253-254 °C. FTIR (KBr, cm⁻¹) v: 3304 (-NH-), 2962 (propyl), 1678 (>C=O) and 1626 (>C=N-); ¹H NMR (CDCl₃, 300 MHz) δ in ppm: 1.0 (t, 6H, -CH₃ propyl, J=7.2Hz), 1.9 (m, 4H, -CH₂-, J=7.2Hz), 2.3 (s, 6H, -CH₃), 4.3 (t, 4H, -OCH₂-, J=6.9 Hz), 7.0 (t, 2H, C₄-thiophene), 7.4 (m, 4H, C₃ and C₅-thiophene). Elemental analysis; C₂₄H₂₈N₄O₄S₃ Calculated C, 54.11%; H, 5.30%; N, 10.52%; S, 18.06%. Found: C, 54.01%; H, 5.22%; N, 10.62%; S, 18.09%. **3,4-Dipropyloxy-N²,N⁵-bis[1-(3-thienyl)ethylidene]thiophene-2,5-dicarbo hydrazide (T₃)**

M.P: 256-257 °C. FTIR (KBr, cm⁻¹) v: 3308 (-NH-), 2969 (propyl), 1675 (>C=O), 1535 (>C=N-); ¹H NMR (CDCl₃, 300 MHz) δ in ppm: 1.06 (t, 6H, -CH₃ of propyl, J=7.2 Hz), 1.88 (m, 4H, -CH₂-), 2.33 (s, 6H, -CH₃), 4.28 (t, 4H, -OCH₂-), 7.31 (d, 2H, C₄-of thiophene, J=16.2), 7.62 (s, 2H, C₂- of thiophene), 7.71 (d, 2H, C₅- of thiophene, J=4.5), 10.13 (s, 2H, -NH-). Elemental analysis data's for C₂₄H₂₈N₄O₄S₃: C, 54.11%; H, 5.30%; N, 10.52%; S, 18.06%. Found: C, 54.02%; H, 5.22%; N, 10.59%; S, 18.15%.

3,4-Dipropyloxy-N²,N⁵-bis[1-(2-bromo-2-thienyl)ethylidene]thiophene-2,5-dicarbohydrazide (T_4)

M.P: 214-215 °C. FTIR (KBr, cm⁻¹) v: 3307 (-NH-), 2967 (propyl), 1677 (>C=O), 1548 (>C=N-). ¹H NMR (CDCl₃, 300 MHz) δ in ppm: 1.0 (t, 6H, -CH₃ propyl, J=7.2 Hz), 1.9 (m, 4H, -CH₂-, J=7.2Hz), 2.3 (s, 6H, -CH₃), 4.3 (t, 4H, -OCH₂-, J=6.9 Hz), 7.0-7.5 (m,4H, C₃ and C₄-thiophene). MS (m/z, %): 691 (M+1, 100), 473 (30), 387 (20). Elemental analysis; C₂₄H₂₆Br₂N₄O₄S₃calcd:C, 41.75%; H, 3.80%; N, 8.11%; S; 13.93%. Found: C, 41.84%; H, 3.87%; N, 8.18%; S; 13.85%.

3. Results and Discussion

The synthesis route of the thiophene derivatives (T_1-T_4) is presented in the Scheme 1. The formation of thiophene derivatives (T_1-T_4) was confirmed by their IR, NMR and mass spectral studies. IR spectra of thiophene derivatives (T_1-T_4) exhibited the absorption band due to N-H in the region 3308-3222 cm⁻¹, n-propyl band at 2969-2962 cm⁻¹, C=O bond at 1678-1641cm⁻¹ along with all other bands. The ¹H-NMR results supports the IR observations. The representative ¹H-NMR spectrum of T_1 is discussed here. The spectrum showed triplet in the region of δ , 0.9-1.06 (J = 7 - 7.2). A multiplet appeared at δ 1.7-1.9 ppm is due to the –CH₂- group. A triplet appeared in the region of δ 4.2 – 4.3 ppm due to protons of –OCH₂- with the coupling constant J = 6.7 - 6.9. A triplet appeared at the region of δ 7.0 - 7.5 due to protons of C₄. A singlet appeared at the region of 8.6 due to protons of -N=CH-. A characteristic singlet appeared at δ 11.2 is assigned to proton of -CONH-. In the compounds (T_1-T_4) , the peak due to azomethine was not observed and a singlet around δ 2.3ppm due to protons of -CH₃ group was observed along with all other functional protons. The mass spectrum of representative compounds T_1 displayed the molecular ion peak m/z (M⁺) at 504. The elemental analysis confirms the purity of the compounds. Synthesis of chemical structures of the compounds T1, T2, T3 and T4 is given in Scheme 1. Individual chemical structure of the compounds T_1 , T_2 , T_3 and T_4 is given in supplementary section (Fig.S1).



Scheme 1. Synthesis of T_1 - T_4 , thiophene based derivatives.

3.1. Photoalignment studies

The UV/Vis absorption spectra of T_1 - T_4 exhibited a peak at 366, 366, 363 and 363 nm, respectively, as shown in Figure 1. Due to the similarity in the chemical structure one can observe similar wavelength for all the reported compounds here.

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Figure 1. Absorption spectra of the compounds (a) T_1 , (b) T_2 , (c) T_3 and (d) T_4 showing absorption peak around ~363-366 nm.

According to the anisotropic response of the bis-hydrazide molecules under the excitation of resonant (with bis-hydrazide molecules) light, photo-stationary orientational states can be expected using proper excitation geometry.

In the present work, the liquid crystal alignment promoted by the alignment layers made from the thiophene derivatives after exposure of the layers with linear polarized UV light for about 15 minutes were investigated. The quality of the obtained liquid crystal alignment in the experimental cells containing PhA layer made of compounds T_1, T_2, T_3 , and T_4 respectively, was studied by means of polarizing microscope. The dark cell image, as shown in Figure 2, corresponds to the cell position between crossed polarizes with the its optic axis oriented along the transmission direction of one of the crossed polarizer whereas the bright image has been taken after rotating the cell at 45^0 .



Figure 2. Photographs of experimental cell, containing PhA layer made from compound T_1 , inserted between crossed polarisers. The cell gap is about 5 μ m and it is filled with the nematic mixture MLC 6873-100 ($\Delta \epsilon$ >0). The preferred alignment direction of the liquid crystal in the cell is oriented at angle 45° with respect to the transmission direction of one of the crossed polarisers (bright state) and 0° with respect to it (dark state). P and A in the diagram represents polarizer and analyser directions.

Materials	Duration of	Photo-	Molecular
used in this	UV exposure	alignment	orientation
study	(min)	results	
T_1	15	Good	Parallel
T_2	15	Good	Perpendicular
T_3	15	Very good	Perpendicular
T_4	15	Weak	Perpendicular

Table 1 Photoalignment promoted by alignment layers made from T_1 - T_4 thiophene based derivatives showing planar alignment with preferred direction parallel to the UV light polarisation plane, for T_1 (without methyl substitution), and perpendicular to it, for T_2 - T_4 (with methyl substitution).

The evaluated quality of the PhA in the cells together with preferred direction of PhA, with respect to the polarization plane of the UV light illumination, is summarized in Table 1. By means of λ first order red plate was found that the alignment layer made by the compound T₁ promoted planar alignment with preferred direction parallel to the UV light polarization plane whereas the other PhA layers made from the compounds T_2 , T_3 and T_4 , respectively, promoted planar alignment but with preferred direction perpendicular to the UV light polarization plane. Except for the compound T_1 all other compounds possess methyl group at the carbon of the HC=N- functional group. Hence, the presence of methyl group seems to be of vital importance for the orientation of liquid crystal alignment direction with respect to UV light polarization plane. Detail discussion about this behavior in which slight modification in the molecular structure results in such drastic change in the PhA properties of the thiophene compounds is given in modelling section of this paper.

During the exposure of thiophene derivatives with linear polarized UV light, their molecules adopt orientation perpendicular to the UV light polarization plane with the molecular axes lying in the plane of the liquid crystal layer (planar alignment). The interactions of thiophene molecules with the liquid crystal molecules are complex due to T-shape of the thiophene molecules. These interactions could generally be characterized by the interplay between two main factors-steric and dipole-dipole interactions. Via steric interactions, the molecules of the thiophene compounds tend to orient liquid crystal molecules, which are in the close contact with the PhA layer, along the thiophene molecule long axis. Steric interactions are short range interactions but their influence on the alignment of the liquid crystal molecules penetrate in the bulk of the liquid crystal layer via elastic forces. In present scenario, however, should be pointed out that there are two alkyl chains in the central part of the thiophene molecules, oriented orthogonally to the molecular axis, which violate the orientation promoted by the steric interactions. Thus in this case, the other long range interactions go to the forefront. These are the dipole-dipole interactions. As it was shown in the works [18] the dipole-dipole interactions are to be addressed not as the interactions between the whole molecules, but as between the localized polar groups of the molecules, which have the zero net charge of the group and the size comparable with the intermolecular distances. The side groups are mobile and thus are capable to orient in one direction, supplying the long-range orientational order with characteristic distance many times greater than the size of the molecule which results in either parallel or perpendicular orientation of the liquid crystal molecules with respect to the molecules of the alignment layer. It provides orientation of the liquid crystal molecules near to the surface of the PhA thiophene layer. Herewith the orientational effect of the dipole-dipole interactions is

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determined by the value of the longitudinal component of the dipole moment of the side groups of the thiophene molecules. Further we have analysed the molecular structures and their impact on the liquid crystal alignment from this point of view using molecular modelling studies.

3.2 Molecular modelling studies

According to modelling results the optimized structures of T_1, T_2, T_3 and T_4 (Fig 3) possess strong dipole moment of 10.5D, 11.2D, 12.4D and 10.8D correspondingly, which are orthogonal to the long molecular axis. The large value of the total molecular dipole moment can be compensated within close molecular neighboring by formation of the two molecule pair with antiparallel orientation of the net dipole moments of the molecules in the pair. The presence of the alkyl chains in the central part of the thiophene molecule, however, hinders the interaction of this part both with the other thiophene molecules, as well as with the liquid crystal molecules. In that case the dipole moments localized on the side groups of the thiophenes [See Figure 4] are important for the long range interaction with liquid crystals.

We conclude that the transverse dipole moment of the side groups is mutually compensated for the T_2 , having too small long range impact on the PhA ability of the alignment layer made from T_2 .



Figure 3. Molecular structures with localized dipole moments of the compounds: a) T_1 , b) T_2 , c) T_3 and d) T_4 . The direction of the UV light polarisation and the promoted liquid crystal alignment by the PhA layers made from these compounds are also depicted. T4 represents very week anchoring energy and difficult to measure and alignment quality also very bad.



Figure 4. Side groups with dipole moments localized within the a) T_1 , b) T_2 , T_3 and T_4 , c) T_1 , T_2 and T_3 , d) T_4 compounds.

Therefore, the steric interactions take over and promote alignment of the liquid crystal molecules along the long molecular axis of the thiophene molecules and thus being oriented perpendicular with respect to polarisation direction of UV light illumination. However, the mutual compensation of the side groups localized transverse dipole moments for the T_1 is lower, enhancing thus the ability of the alignment layer made from this compound to promote liquid crystal alignment due to the long range dipole-dipole interactions. Thus the PhA layer made from T_1 is capable to orient nematic liquid crystals with positive dielectric anisotropy along direction perpendicular to the long molecular axis of the thiophene molecule. This alignment direction, however, coincides with the polarisation direction of the UV light.

Compare the side groups shown on Figure 4a and 4b, the presence of the CH_3 radical donate the electron density thus increasing the dipole moment of the group 2.16D and 2.66D, correspondingly. It explains the difference of the localized transverse dipole moments of these side groups and its' ability to compensate the transverse dipole moment localized in the terminal side group (Fig. 4c) of the compound T_1 (Fig.3a) and T_2 (Fig.3b).

Consider the longitudinal orientation of the side group in Fig 4c within the T_3 compound (Fig.3c). In contrast to the compound in Fig.3a the presence of the longitudinal dipole moment localized on the side group explains the ability to orient the nematic liquid crystal with positive dielectric anisotropy along the molecular axis of the thiophene due to the long range dipole-dipole interactions. The latter results in that the PhA layer made from T₁ compound promote liquid crystal alignment being perpendicular to the UV light polarisation direction. The side group in Fig.4d of the T_4 compound (Fig.3d) has negatively charged Br atom in the outside of the molecule. The terminal radicals of such molecular structures are likely to repel, which prevent from formation of anisotropic rotational distribution of thiophene molecules in the PhA layer. Similar behavior was observed for SD2 dye with CF3 terminal radicals [19]. Thus the long range averaged dipole-dipole interactions of the T₄ compound layer are not capable to form any photoalignment preferred direction of the liquid crystal. Thus T_4 compound does not possess such a liquid crystal photoalignment ability as the other thiophene derivatives.

By incorporating different functional groups in the molecular structure or by increasing the anisotropy in this structure one can increase the stability of the PhA. Moreover, by including photoreactive mesogenic molecules in the PhA layer made from thiophenes derivatives, the temperature stability of the PhA will substantially be increased.

In this study, the intensity of the mercury light is low. Therefore, it takes much longer time to obtain PhA of the nematic liquid crystal with this kind of thiophenes. Hence, increasing the illumination power will reduce the exposure time necessary to obtain good PhA quality. Moreover, with subsequent ozone treatment of the substrates before spin coating with the solution containing the thiophene material, it is found that the quality of PhA, promoted by these materials, is improved drastically.

4. Conclusion

Our study demonstrated that small changes in the molecular structure of the thiophene material, the PhA layer is made of, may have strong impact on the alignment ability of this layer. However, these modification of the molecular structure have to be of such nature that they change the balance in the interactions resulting PhA of the nematic molecules, as in our case. Inclusion of methyl group in the thiophene compounds under study caused turning the preferred direction of alignment the nematic liquid crystal promoted by the thiophene PhA layer from parallel with respect to the polarisation of UV light, for the thiophene compound without methyl group, to perpendicular to it, for the thiophenes compound with methyl group. Advancing the knowledge about the relations between molecular structure of the compounds, the liquid crystal alignment layers are made of, will enable to design new PhA materials and to tailor their alignment characteristics.

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Notes and references

^aBMS R and D Centre, BMS College of Engineering, Basavanagudi, Bangalore, 560078, India.

^bInstitute of Chemistry of New Materials, NAS of Belarus, Minsk, Belarus.

^cDept of Chemistry, National Institute of Technology, Suratkal, Karnataka, India.

^dLiquid Crystal Physics Group, University of Gothenburg, Gothenburg, Sweden

*Author for correspondence: <u>murthyhegde@gmail.com</u>

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