Theoretical investigation on absorption spectral profile of tetrazole liquid crystals: Hexyl, nonyl end groups and solvent effects

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Abstract. In this article, a theoretical investigation on absorption spectral profile of tetrazole liquid crystals 4-[(2-alkyl)-2H-tetrazol-5-yl] phenyl 4-alkyloxybenzoates (nTPmB; with n=m=6, 9) has been carried out. The hexyl, nonyl, and solvent (DMSO) effects on absorption spectral profiles have been investigated using the CNDO/S, and INDO/S methods. Population analysis of these molecules in the gaseous state has been performed by generalized atomic polar tensor (GAPT) charge distribution scheme for AM1, PM3, MNDO, CNDO/S, and INDO/S methods. The observed \( \pi \rightarrow \pi^* \), and \( n \rightarrow \pi^* \) electronic transitions have been reported. The hexyl, nonyl end groups and solvent effects on absorption profiles have been discussed to analyse the photo stability of the molecules. Further, a through comparative analysis of reactivity descriptors has been made. The reported data may offer an insight in determining the end use of compounds.

1. Introduction
Long-range orientation ordered liquid crystals (LCs) are superior over normal crystals due to some of its special properties from application point of view [1]. LCs may contain various kinds of functional molecular systems which are electronegative [2, 3] in nature. LCs are structurally flexible enough so that it can be mixed with other compatible substances in any proportion by varying molecular structure, reorientation and improving physical properties like photo sensitivity and stability, optical behaviour, absorption of radiation. Qualitative character in the field of optics multiply its application broadly in the area of photonics, manufacture of photo sensitive devices, optical switching and signal processor. Remarkable changes will appear in properties of LCs due to several molecular arrangements with complex stratified structure.

Understanding of spectroscopic properties is compulsory for checking the viability of LCs for photonic applications [4, 5]. Spectroscopy plays vital role for observation of properties of number of anisotropic molecular compounds. It can characterize LC molecules and find their structure on the basis of absorption spectrum as a function of specific wavelength and frequency. Significance of absorption spectrum demonstrates the radiation available for absorption for the interacting sample. The resultant spectral profile acts as a fingerprint from which data are matched with reference parameters if available in the literature. Absorption spectrum gives more accurate results in a simpler way. Qualitatively it can measure the concentration of a molecule in a solution because molecules absorb energy at a specific wavelength [6]. Besides that, polarization of the electronic transition in UV and visible radiation and dipole-dipole interaction in intermolecular level will be observed. From the absorption spectra stable region can be analysed at particular wavelength, frequency and corresponding energy can be known. As the absorbed radiation transferred into heat and gradually warm up the LC molecules [7], parameters like order parameter, dielectric constant, optical anisotropy will be affected due to the absorption of certain frequency of radiation.

This article has been intended to offer a comparative picture of UV-Visible absorption spectral parameters of \( nTPmB \) (n=m=6, 9) molecules using the CNDO/S [8, 9], and INDO/S [10] methods along with CIS method [11] using the semiempirical ZINDO [12-14] Hamiltonian for excited states calculation. Charge transfer process of the molecules in the gaseous state has been performed by generalized atomic polar tensor (GAPT) charge distribution scheme for AM1, PM3, MNDO,
CNDO/S, and INDO/S methods. The shifts in absorption bands have been discussed. The spectral parameters have been reported to explain the photo sensitivity of the compounds. The LC behaviour and the transition temperatures of the compounds have been reported [15].

2. Methodology
The CNDO/S and INDO/S are versions of the ordinary CNDO, INDO procedures reparametrized to reproduce experimental excitation energies. The SCF step is frequently followed by limited configuration interaction (CI) calculations over a truncated set of singly excited configurations. In both the methods, the wave functions of the ground, and electronically excited states of $\pi\pi^*$-type have been once investigated in the one-configurationally approximation. The UV-Visible absorption spectrum has been calculated using the CI method on the basis of the obtained multi electron wave functions.

The CNDO/S and INDO/S methods including all valence electrons along with configuration interaction analysis have been used to calculate the UV-Visible absorption spectra of the molecules. A revised version of QCPE program 174 by Jeff Reimers, University of Sydney, and co-workers have been used for these calculations [16]. The general structural parameters of the systems such as bond lengths, and bond angles have been taken from the published crystallographic data [15]. The electrochemical properties have been estimated using the formulae reported in Table 4.

3. Results and Discussion
The molecular structures of 6TP6B and 9TP9B that have been constructed based on published crystallographic data [15] have been shown in Figure 1. Atomic net charges have been calculated using AM1, PM3, MNDO, CNDO/S, INDO/S schemes have been reported in Table 1 and 2 for 6TP6B and 9TP9B respectively. The AM1, PM3, and MNDO charges have been obtained by MOPAC calculations available via VEGA ZZ package [17]. The atomic partial charge analysis and intermolecular charge transfer of the compounds have been analyzed as given below.

Figure 1 Molecular structures of (A) 6TP6B and (B) 9TP9B compounds
3.1. Atomic partial charge analysis

The atomic charges of nTPmB (n=m=6, 9)molecules have been reported in Table 1 and 2. From the tables, discrepancies may be observed in terms of individual atomic partial charges. However, much agreement has found out in general in case of group charges. Carbon and nitrogen atoms carry both positive and negative charges. Most of the carbon atoms in the end chain carry negative charge for 6TP6B. Most negative charged atom is O_{32}. The next maximum negative charged atoms are O_{33} and O_{31} respectively. The maximum positive charge acquired by C_{1} followed by C_{1} and C_{12}. Similarly, C_{2} contain maximum positive charge for 9TP9B molecule. Next two maximum positive charged atoms are C_{1} and C_{12}. O_{38} is the most negative charged atom followed by O_{39} and N_{33}. All the five different schemes are in agreement in estimating the atomic partial charges. Hence, the intermolecular charge transfer is stronger in both the molecules between side to aromatic groups and end to aromatic groups.

From Table 1 and 2, it may be observed that the strongest positive and negative charges in both molecules are nearly same. Hence, appreciable difference in terms of phase transition temperature may not be found. This is in accord with literature details [15].

Table 1 Interatomic charge distribution for 6TP6B molecule (heavy atoms) using CNDO/S, INDO/S, AM1, PM3, and MNDO methods.

| S.No. | Atom | CNDO/S | INDO/S | AM1 | PM3 | MNDO |
|-------|------|--------|--------|-----|-----|------|
| 1     | C_{1} | 0.199  | 0.187  | -0.092 | -0.056 | -0.019 |
| 2     | C_{2} | 0.406  | 0.452  | 0.363  | 0.433  | 0.417 |
| 3     | C_{3} | 0.004  | 0.008  | -0.022 | -0.029 | -0.020 |
| 4     | C_{4} | -0.017 | -0.016 | -0.083 | -0.052 | -0.006 |
| 5     | C_{5} | -0.040 | -0.024 | -0.144 | -0.124 | -0.073 |
| 6     | C_{6} | 0.146  | 0.147  | 0.082  | 0.096  | 0.124 |
| 7     | C_{7} | -0.044 | -0.028 | -0.144 | -0.120 | -0.073 |
| 8     | C_{8} | -0.015 | -0.013 | -0.080 | -0.050 | -0.001 |
| 9     | C_{9} | -0.017 | -0.005 | -0.160 | -0.176 | -0.132 |
| 10    | C_{10}| 0.003  | 0.009  | -0.039 | -0.009 | 0.020 |
| 11    | C_{11}| -0.060 | -0.037 | -0.177 | -0.162 | -0.098 |
| 12    | C_{12}| 0.160  | 0.162  | 0.123  | 0.132  | 0.168 |
| 13    | C_{13}| -0.072 | -0.048 | -0.229 | -0.208 | -0.148 |
| 14    | C_{14}| -0.003 | 0.001  | -0.027 | -0.001 | 0.032 |
| 15    | C_{15}| 0.040  | 0.068  | 0.009  | -0.035 | 0.202 |
| 16    | C_{16}| -0.044 | -0.019 | -0.178 | -0.119 | -0.032 |
| 17    | C_{17}| -0.054 | -0.027 | -0.162 | -0.107 | -0.009 |
| 18    | C_{18}| -0.057 | -0.029 | -0.157 | -0.101 | -0.007 |
| 19    | C_{19}| -0.057 | -0.030 | -0.158 | -0.098 | -0.022 |
| 20    | C_{20}| -0.097 | -0.052 | -0.210 | -0.109 | 0.029 |
| 21    | C_{21}| 0.054  | 0.102  | -0.024 | 0.055  | 0.180 |
| 22    | C_{22}| -0.048 | -0.021 | -0.161 | -0.121 | -0.010 |
| 23    | C_{23}| -0.058 | -0.030 | -0.158 | -0.100 | -0.006 |
| 24    | C_{24}| -0.055 | -0.026 | -0.157 | -0.102 | -0.007 |
| 25    | C_{25}| -0.056 | -0.028 | -0.159 | -0.106 | -0.021 |
| 26    | C_{26}| -0.099 | -0.055 | -0.211 | -0.107 | 0.029 |
| 27    | N_{27}| -0.251 | -0.251 | -0.057 | -0.210 | -0.095 |
| 28    | N_{28}| 0.068  | 0.148  | -0.157 | 0.221  | -0.174 |
| 29    | N_{29}| -0.077 | -0.100 | 0.018  | -0.121 | 0.019 |
| 30    | N_{30}| -0.218 | -0.225 | -0.106 | -0.091 | -0.137 |
| 31    | O_{31}| -0.242 | -0.272 | -0.236 | -0.222 | -0.283 |
| 32    | O_{32}| -0.448 | -0.510 | -0.336 | -0.364 | -0.339 |
| 33    | O_{33}| -0.260 | -0.309 | -0.208 | -0.185 | -0.277 |
Table 2 Interatomic charge distribution for 9TP9B molecule (heavy atoms) using CNDO/S, INDO/S, AM1, PM3, and MNDO methods.

| S.No. | Atom | Atomic Charges          |
|-------|------|-------------------------|
|       |      | CNDO/S | INDO/S | AM1  | PM3  | MNDO |
| 1     | C1   | 0.202  | 0.188  | -0.090 | -0.057 | -0.010 |
| 2     | C2   | 0.407  | 0.453  | 0.363  | 0.433  | 0.417  |
| 3     | C3   | 0.005  | 0.009  | -0.021 | -0.027 | -0.022 |
| 4     | C4   | -0.013 | -0.011 | -0.081 | -0.050 | -0.006 |
| 5     | C5   | -0.043 | -0.028 | -0.144 | -0.121 | -0.075 |
| 6     | C6   | 0.145  | 0.146  | 0.081  | 0.094  | 0.124  |
| 7     | C7   | -0.036 | -0.020 | -0.144 | -0.117 | -0.072 |
| 8     | C8   | -0.017 | -0.016 | -0.083 | -0.054 | -0.005 |
| 9     | C9   | -0.015 | -0.003 | -0.159 | -0.172 | -0.132 |
| 10    | C10  | -0.005 | -0.001 | -0.027 | -0.003 | 0.031  |
| 11    | C11  | -0.065 | -0.042 | -0.229 | -0.205 | -0.148 |
| 12    | C12  | 0.156  | 0.160  | 0.123  | 0.130  | 0.168  |
| 13    | C13  | -0.058 | -0.036 | -0.176 | -0.158 | -0.098 |
| 14    | C14  | 0.001  | 0.008  | -0.040 | -0.011 | 0.021  |
| 15    | C15  | 0.038  | 0.064  | 0.011  | -0.039 | 0.203  |
| 16    | C16  | -0.046 | 0.022  | -0.174 | -0.122 | -0.036 |
| 17    | C17  | -0.058 | -0.032 | -0.158 | -0.098 | -0.008 |
| 18    | C18  | -0.058 | -0.031 | -0.157 | -0.101 | -0.008 |
| 19    | C19  | -0.059 | -0.032 | -0.157 | -0.101 | -0.008 |
| 20    | C20  | -0.059 | -0.030 | -0.157 | -0.102 | -0.007 |
| 21    | C21  | -0.058 | -0.030 | -0.157 | -0.102 | -0.007 |
| 22    | C22  | -0.058 | -0.031 | -0.158 | -0.097 | -0.021 |
| 23    | C23  | -0.098 | -0.053 | -0.210 | -0.109 | 0.029  |
| 24    | C24  | 0.052  | 0.100  | -0.023 | 0.053  | 0.180  |
| 25    | C25  | -0.049 | -0.023 | -0.165 | -0.115 | -0.017 |
| 26    | C26  | -0.060 | -0.031 | -0.156 | -0.098 | -0.011 |
| 27    | C27  | -0.059 | -0.031 | -0.157 | -0.101 | -0.008 |
| 28    | C28  | -0.059 | -0.032 | -0.157 | -0.101 | -0.008 |
| 29    | C29  | -0.059 | -0.031 | -0.157 | -0.101 | -0.008 |
| 30    | C30  | -0.058 | -0.029 | -0.157 | -0.102 | -0.007 |
| 31    | C31  | -0.057 | -0.030 | -0.158 | -0.097 | -0.021 |
| 32    | C32  | -0.097 | -0.053 | -0.210 | -0.109 | 0.029  |
| 33    | N33  | -0.256 | -0.255 | -0.060 | -0.213 | -0.096 |
| 34    | N34  | 0.062  | 0.139  | -0.155 | 0.230  | -0.175 |
| 35    | N35  | -0.067 | -0.091 | 0.017  | -0.124 | 0.019  |
| 36    | N36  | 0.224  | -0.231 | -0.108 | -0.090 | 0.139  |
| 37    | O37  | -0.242 | -0.272 | -0.236 | -0.220 | -0.283 |
| 38    | O38  | -0.451 | -0.513 | -0.336 | -0.363 | -0.339 |
| 39    | O39  | -0.264 | -0.314 | -0.208 | -0.187 | -0.278 |

3.2. Absorption spectral profile
(a) Pure compounds of 6TP6B and 9TP9B:
The absorption spectra of nTPmB (n=m=6, 9) pure molecules using CNDO/S, and INDO/S methods have been shown in Figure 2 and 3 respectively. CNDO/S method estimates two band spectra whereas; INDO/S method estimates one band spectra. The 6TP6B and 9TP9B molecules exhibits absorption maxima at 240.42nm, 238.67nm (CNDO/S), and 249.22nm, 248.63nm (INDO/S) respectively. However, the extinction coefficient has been decreased from 0.80 to 0.79 (CNDO/S) and 1.11 to 1.01 (INDO/S) respectively. These bands arises from the HOMO→LUMO transition, and is assigned as π→π* transition. The other absorption bands corresponding to the remaining wavelengths
in UV region also indicate the more numbers of $\pi\rightarrow\pi^*$ transitions at other wavelengths. Therefore, both methods are in agreement with each other by exhibiting blue-shift of wavelength, and hypochromic effect when hexyl end group is replaced by nonyl end group.

The spectral parameters of $nTPmB$ ($n=m=6, 9$) pure molecules have been reported in Table 3. The above mentioned blue-shift is possible due to the excitation of the electron that causes an increment in transition energies (Table 3). Therefore, this makes the absorption band to poor interaction electrostatically. From the literature, it has been observed that the 9TP9B exhibits little higher transition temperature [15] compared to 6TP6B. So, the high phase stability of 9TP9B plays a vital role for increment in the transition energies. This leads to differences in charge distribution of the compound, and a reduced delocalization of electrons. Hence, it may be concluded that the ground, and excited $n\rightarrow\pi^*$ transitions are not visualized due to the less molecular rigidity offered by the ring system.

b) Solvent (DMSO) effect
The spectral parameters of $nTPmB$ ($n=m=6, 9$) molecules in DMSO are reported in Table 3 using CNDO/S, and INDO/S methods. CNDO/S method estimates two band spectra of 6TP6B in DMSO with 257.42nm as absorption wavelength, and INDO/S method estimates four band spectra with 321.87nm as absorption wavelength in DMSO (fig 4 and fig 5). Therefore, the solvent causes a red-shift of wavelength compared to pure molecules (Table 3). Further, hypochromic effect has been observed for 6TP6B molecule in DMSO. Hence, it may be understood from the spectral parameters reported in Table 3 that the UV stability of 6TP6B is more compared to 9TP9B in pure form. The DMSO effect does not alter the UV stability of 6TP6B as it is evident from Table 3. Moreover, increment of end chains from hexyl to nonyl groups does not alter the nature of shift of wavelength in DMSO. But the solvent enhances the UV stability of individual compounds from its pure form to solvent. Further, both methods predict a lesser band gap for 6TP6B molecule which concludes the conductivity of 6TP6B.
Table 3. The absorption bands (AB), extinction coefficients (EC), Oscillator strength (f), Vertical transition energy (E_V), dipole moment (µ), HOMO (H), LUMO (L) energies, and the band gap (E_g=E_{LUMO}-E_{HOMO}) values of nTPmB (n=m=6, 9) pure molecules and in DMSO using CNDO/S, and INDO/S methods.

| Molecule/Method | AB/ nm | EC* | f   | E_V/ eV | µ/D | H= | L= | E_g |
|-----------------|--------|-----|-----|--------|-----|-----|-----|------|
| 6TP6B CNDO/S Pure | 240.42 | 0.80 | 0.51 | 5.14   | 6.81| -9.13 | -1.53 | 7.60 |
| DMSO            | 257.42 | 0.35 | 0.35 | 4.68   | 11.93|
|                 | 286.13 | 0.12 | 0.12 | 4.33   | 7.06 |
| H= -9.13        | L= -1.53 |  |  |  |  |
| 6TP6B DMSO      | 264.45 | 0.35 | 0.35 | 4.68   | 11.93|
|                 | 286.13 | 0.12 | 0.12 | 4.33   | 7.06 |
| H= -9.13        | L= -1.53 |  |  |  |  |
| 9TP9B CNDO/S Pure | 248.63 | 1.01 | 0.30 | 4.95   | 7.68| -7.87 | -0.41 | 7.46 |
| DMSO            | 238.67 | 0.79 | 0.68 | 5.16   | 5.94|
|                 | 263.28 | 0.37 | 0.37 | 4.70   | 11.66|
|                 | 205.27 | 0.62 | 0.55 | 6.02   | 4.13|
|                 | 238.08 | 0.30 | 0.30 | 5.21   | 9.13|
|                 | 683.22 | 0.11 | 0.11 | 1.82   | 5.80|
|                 | 789.07 | 0.20 | 0.21 | 1.58   | 6.04|
| H= -7.87        | L= -0.41 |  |  |  |  |
| 9TP9B DMSO      | 213.47 | 0.05 | 0.05 | 5.81   | 4.64|
|                 | 301.95 | 0.26 | 0.26 | 4.11   | 8.78|
|                 | 396.87 | 0.02 | 0.02 | 3.12   | 6.10|
|                 | 454.29 | 0.34 | 0.31 | 2.72   | 5.99|
|                 | 478.32 | 0.14 | 0.14 | 2.59   | 5.68|
| H= -7.92        | L= -0.39 |  |  |  |  |

*EC unit: 10^4 dm^3 mol^-1 cm^-1  **Bold**value represents UV absorption maxima

Figure 4 Absorption spectra of 6TP6B and 9TP9B molecules in DMSO using CNDO/S Method

Figure 5 Absorption spectra of 6TP6B and 9TP9B molecules in DMSO using INDO/S Method
(c) Electrochemical properties
The electrochemical properties of the \(nTPmB\) \((n=m=6, 9)\) molecules using CNDO/S, INDO/S methods have been reported in Table 4. The estimated energy gap and chemical hardness values offer an understanding of the chemical stability of the compounds. The larger energy gap indicates the larger kinetic stability in accordance with the principle of softness-hardness. In general, the more energy gap of the molecule offers more hardness, and also provides higher thermal and kinetic stability. The smaller gap lowers the kinetic stability and offers higher chemical reactivity. The parameter \(\Delta N_{\text{max}}\) reveals the propensity of the molecule to get additional electronic charge from the environment. It has been observed from the Table that both molecules exhibit same values of maximum charge transfer. This indicates the almost similar charge distribution behaviour of the molecules which is in agreement with the partial charge analysis (section 3.1).

Further, it may be observed from Table 4 that almost all parameters increase from hexyl to nonyl group, and both methods are exhibits good agreement in estimating all the parameters.

Table 4 Calculated values of ionization energy \(I=-(E_H)\), electron affinity \(A=-(E_L)\), electron negativity \(\chi=(I+A)/2\), chemical hardness \(\eta=(I-A)/2\), electronic chemical potential \(\mu=-((I+A)/2\), electrophilic index \(\omega=\mu^2/\eta\), and softness \(S=1/\eta\), maximum charge transfer \(\Delta N_{\text{max}}=-(\mu/\eta)\), of \(nTPmB\) \((n=m=6, 9)\) molecules using CNDO/S, and INDO/S methods.

| Molecule | Parameter | CNDO/S method | INDO/S method |
|----------|-----------|---------------|---------------|
| 6TP6B    | I/eV      | 9.13          | 7.87          |
|          | A/eV      | 1.53          | 0.41          |
|          | \(\chi/eV\) | 5.33          | 4.14          |
|          | \(\eta/eV\) | 3.80          | 3.73          |
|          | \(\mu/eV\) | -5.33         | -4.14         |
|          | \(\omega/eV\) | 7.47          | 4.60          |
|          | \(S/eV^{-1}\) | 0.26          | 0.27          |
|          | \(\Delta N_{\text{max}}\) | 1.40          | 1.11          |
| 9TP9B    | I/eV      | 9.19          | 7.92          |
|          | A/eV      | 1.56          | 0.39          |
|          | \(\chi/eV\) | 5.37          | 4.15          |
|          | \(\eta/eV\) | 3.81          | 3.76          |
|          | \(\mu/eV\) | -5.37         | -4.15         |
|          | \(\omega/eV\) | 7.57          | 4.58          |
|          | \(S/eV^{-1}\) | 0.26          | 0.26          |
|          | \(\Delta N_{\text{max}}\) | 1.41          | 1.10          |

4. Conclusions
1. The strongest positive and negative charges in both molecules are nearly same. Hence, appreciable difference in terms of phase transition temperature may not be found. This is in accord with literature details.
2. Both methods are in agreement with each other by exhibiting blue-shift of wavelength, and hypochromic effect when hexyl end group is replaced by nonyl end group in pure form.
3. The UV stability of 6TP6B is more compared to 9TP9B in pure form. The DMSO effect does not alter the UV stability of 6TP6B. But the solvent enhances the UV stability of individual compounds from its pure form to solvent.

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