

APPLICATION OF A NOVEL SYMMETRIC BENZOPHENONE DERIVATIVE SCHIFF BASE IN LYOTROPIC MEDIA AND SPECTROSCOPIC PROPERTIES

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The structural and spectroscopic properties of a new –ONNO– type Schiff base were analyzed. The compound 6,6'-((1*E*,1'*E*)-(hexane-1,6-diylbis(azaneylylidene))bis(phenylmethaneylylidene))bis(3-(octyloxy) phenol) was synthesized by condensing a diamine and a ketone in tetrahydrofuran, resulting in a high yield. The symmetric Schiff base, in which both amine ends converted to the imine structure, was examined using XRD, NMR, IR and UV-Vis spectroscopies. The theoretical calculations were done successfully using DFT approach at 6-31G(*d,p*) basis set to investigate the properties of the title compound that cannot be studied by experimental analyses. NBO analysis was used to study hyper-conjugative interactions involving the overlap of σ or π electrons and electron density between adjacent atoms and to determine the stabilization energy. The DFT theoretical parameters and XRD experimental parameters were compared and showed good agreement. 2D fingerprint and 3D Hirshfeld surface plots were obtained to determine the intermolecular interactions. The features of the optimized structure were investigated by several analyses such: NBO, Frontier molecular orbitals, ESP, MEP and ECT which cannot be studied by theoretical methods. The UV-Vis spectroscopy was used to investigate the interaction of the synthesized benzophenone Schiff base compound with lyotropic media. The synthesized compound is significantly compatible with the prepared lyotropic medium due to its highly symmetrical and amphiphilic structure.

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INTRODUCTION

In living organisms and including natural-unnatural product areas the most important scaffolds are heteroaromatic molecules with excellent chemical, temperature, or UV light selectivity. This enables the development of steps that mimic nature in many areas by designing heteroaromatic molecules containing desired and controllable functional groups according to need [1, 2]. Benzophenone is a natural heteroaromatic molecule motif, known for its remarkable chemical stability and

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broad resonances. In many areas, benzophenone-derived compounds are encountered in many areas that allow for different uses such as photoinitiator, and enantiomeric separation. But the most attractive area is organic π -conjugated push-pull molecules due to electron-deficient structure in recent years [3, 4]. An important aspect of benzophenone-derived compounds that attracts attention is their similarity to some important biochemical structures for living beings, and this similarity allows the production and examination of pharmacological agents that can affect many diseases such as cancer [5]. Another notable aspect of benzophenone derivatives, such as those used in cosmetics and polymers, is their susceptibility to UV rays, which is particularly significant in today's development areas. Especially 2-hydroxy-4-alkyloxy derivatives are used as protective agents in many medicinal applications [6]. To enhance biologically effective compound formation, the synthesis of an imine bond through the reaction of an amine is a commonly employed method. The formation of imine bonds is a common method to obtain nitrogen-based heteroaromatic molecules, increasing biological efficiency, pH sensitivity, and reducing electrophilicity [7]. In literature, it was reported that some hydroxybenzophenone derivatives exhibit cytotoxic effects, efficient bio-efficacy, and the ability to cleavage and bind with DNA [6, 8-10].

Stability, order and symmetry are not just interesting features of nature but also fundamental principles in any future fields, such as biomimetics. The mechanism of liquid crystal formation depends especially on the molecular order and symmetry and for these reasons, liquid crystals attract a lot of attention in several fields. Intermolecular interaction in liquid crystals is one of the important factors that enable self-organization and in this regard, it becomes a specific area used in the investigation of guest-host interaction in isotropic-anisotropic solution environments [11]. There are very few studies in the literature examining the interaction between a lyotropic liquid crystal (LLC) and a biological molecule. One of these notable studies was carried out with POM and ion density measurements to investigate their interaction with DNA. As a result, it was stated that disrupted microscopic texture and similar thermal and potential ion carrier properties were determined [12]. This study aims to examine the synthesis and characterization of a new tetra-dentate Schiff base, which is stable with its different functional groups and high conjugation and attracts attention with its electro-optical properties. It can also serve as a foundation for technological and biological studies, and for investigating the interaction between lyotropic media and Schiff bases. The synthesized molecule was characterized by X-ray, FTIR, ^1H and ^{13}C NMR, and UV-Vis spectroscopies. On the other hand, the synthesized compound has both an apolar alkyl chain and polar functional groups. In light of these properties, it was investigated whether the synthesized compound is suitable for liquid crystal applications in lyotropic media. A cholesteric lyotropic phase was used as a liquid crystal media, and in this target, decylammonium chloride (DACl)/KCl/H₂O/S(-)-Limonene system was used. The synthesized Schiff base was then examined in a lyotropic system by polarized optical microscope (POM) and UV-Vis spectroscopy.

EXPERIMENTAL

Experimental equipment and materials. The used chemicals were purchased from Sigma-Aldrich with analytical grade. Electrothermal-IA9200 was used to determine the melting point. A Vertex 80 V Bruker FTIR spectrometer in the ATR model was used to study the FTIR spectra. NMR spectra were obtained in DMSO-d₆ with TMS as the internal standard by a Bruker Ultra Scield Plus, 500 MHz. The spectra of UV-Vis. were gained through a GBC CINTRA 20 UV-Vis. spectrometer with a 1 cm length quartz optical cell. The UV-Vis spectrum of the synthesized Schiff base was obtained in ethanol and acetonitrile ranging from 200 nm to 800 nm at room temperature. 1.10^{-5} M of Schiff base solutions were used. LLC samples were studied with Nikon Eclipse E400 Polarized optical microscope (POM) and Linkam TP94 hot stage at 25 °C and 37 °C. LLC samples were also analyzed by UV-Vis. spectrometer at temperatures of 25 °C and 37 °C, and pH 7.4. UV-Vis spectra were obtained in the range of 200-1000 nm.

Synthesis of Schiff base ligand. 6,6'-((1*E*,1'*E*)-(hexane-1,6-diylbis(azaneylylidene))bis(phenylmethaneylylidene))bis(3-(octyloxy)phenol) was obtained by traditional method. 1,6-hexane diamine and 2-hydroxy-4-octyloxybenzophenone were used to obtain the title compound. A solution of 1,6-hexane diamine (0.009 mmol, 1.050 mg) in 20 mL THF and 2-hydroxy-4-octyloxybenzophenone (0.018 mmol, 5.880 mg) in 20 mL THF was mixed dropwise to a stoichiometric ratio of

2:1 [13]. The obtained reaction mixture was stirred for 18 h under reflux. The yellow crystal collapsed in the reaction mixture and separated after the end of the reaction. The obtained compound was washed with ethanol and recrystallized with ethanol at room temperature. The synthesized compound was obtained with a high yield of 87%. The determined melting point of the compound is 352 K and the structure of the synthesized compound is illustrated in Fig. 1.

FTIR (cm^{-1}): 3027 ($\nu\text{C-H}$ aromatic), 2923-2852 ($\nu\text{C-H}$ aliphatic), 2500 (νCOH), 1605 ($\nu\text{C=N}$), 1590-1515 ($\nu\text{C=C}$), 1280 (νCO), ^1H NMR (ppm): δ 15.93 (OH), 7.49-6.16 (Ar-H), 3.91 (OCH_2), 3.31 (NCH_2), 1.86-0.84 ($\text{OCH}_2\text{HC}_2\text{CH}_3$), ^{13}C NMR (ppm): δ 173.84 (C=N), 163.08 (COH), 133.31-127.56 (aromatic C=C), 67.93 (NCH_2), 48.12 (OCH_2), 14.40-31.67 (CH_2CH_3), UV-Vis (ethanol, nm): 212 ($\pi\text{-}\pi^*$ benzene), 300 ($\pi\text{-}\pi^*$ imine), 383 ($n\text{-}\pi^*$ imine).

XRD Analysis. Crystallographic data of the single crystal were recorded on Bruker D8 Venture Photon 100 CMOS diffractometer at a temperature of 100 K using graphite-monochromated MoK_α radiation in f and w scans mode ($\lambda = 0.71073 \text{ \AA}$). The structure of the crystal was solved by direct methods in SHELXS [14] and refined through full-matrix least squares methods using SHELXL [15], performed on the WinGX [16] program suite. The molecular structure figures were prepared with the help of ORTEP-3 [17] and Mercury [18] programs. All non-hydrogen atoms were refined anisotropically, whereas the hydrogen atoms were included without refining. Crystallographic data results are shown in Table 1. The crystallographic information and final refinement parameters of the title compound can be obtained from Cambridge Crystallographic Data Centre (CCDC NO: 2285285).

Computational procedure. DFT calculations were conducted to explore the electronic structure and predict the chemical and physical properties that cannot be determined through experimental methods. The geometry of the compound was fully optimized by DFT approach at B3LYP/6-31G(*d,p*) level of theory. All calculations, including the geometry optimization, were performed in the gas phase, whereas the experimental data were obtained in the solid phase. All computations were performed using the Gaussian'16 program package [19] on a supercomputer cluster housed at the National Center for High Performance Computing (UHeM) at Istanbul Technical University, Türkiye. The calculated electron-density plots were generated by using GaussView 6.0 program [20].

Preparation of LLC Media. The preparation of the LLC was carried out according to the steps mentioned in our previous study [21]. Isotrope, nematic and cholesteric phases obtained with DACI/KCl/ H_2O /S(-)-Limonene compounds. To prepare LLC, different amounts of DACI/KCl/ H_2O /S(-)-Limonene components were weighed and heated at 50°C and centrifuged until obtaining a homogeneous system. The synthesized Schiff base was soluted in pure S(-)-Limonene in the range of $7.00 \cdot 10^{-5}$ - $2.25 \cdot 10^{-3}$ M. Phases of LLC with and without Schiff base were analyzed with a polarized optical microscope. At 25°C and 37°C , UV-Vis. spectra were obtained in the range of 200-1000 nm. The same spectra also were obtained at pH = 7.4.

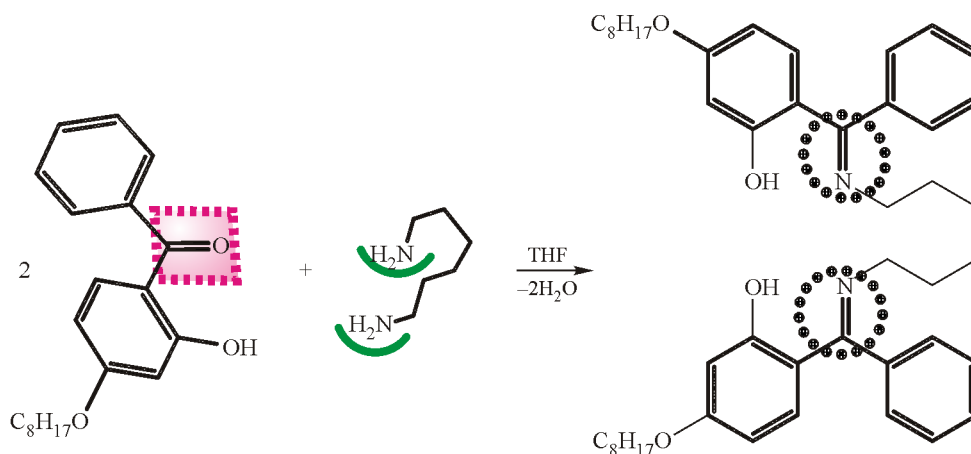


Fig. 1. The synthesis of the benzophenone derivative Schiff base.

TABLE 1. Experimental XRD Details of the Title Compound

Parameter	Data
CCDC number	2285285
Chemical formula	C ₄₈ H ₆₄ N ₂ O ₄
Formula weight	733.01
Wavelength, Å	MoK _α radiation, 0.71073
Temperature, K	100
Crystal system, Space group	Orthorhombic, <i>Pccn</i>
Crystal color	Yellow
<i>a</i> , <i>b</i> , <i>c</i> , Å	15.1474(5), 26.6737(11), 10.3762(4)
Volume, Å ³	4192.4 (3)
<i>Z</i>	4
Density, g/cm ³	1.161
μ, mm ⁻¹	0.07
Absorption correction	Multi-scan, SADABS2016/2 (Bruker AXS Inc.)
<i>F</i> ₀₀₀	1592
Diffractionmeter/ meas. meth.	Bruker D8 Venture Photon 100 CMOS, <i>f</i> and <i>w</i> scans
θ range for data collection, deg	2.5 ≤ θ ≤ 28.3
Index ranges	−18 ≤ <i>h</i> ≤ 20, −35 ≤ <i>k</i> ≤ 30, −13 ≤ <i>l</i> ≤ 13
<i>T</i> _{min} , <i>T</i> _{max}	0.685, 0.746
Reflections collected	35943
Independent/observed reflections	5227, 3812
<i>R</i> _{int}	0.065
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0552, <i>wR</i> ₂ = 0.1183
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0844, <i>wR</i> ₂ = 0.1302
Data/restraints/parameters	5227/0/246
Goodness of fit on <i>F</i> ²	1.03
Δρ _{max} , Δρ _{min} , e/Å ³	0.28, −0.35

RESULTS AND DISCUSSION

Characterization of Schiff Base. A symmetric Schiff base derivative of benzophenone, with high conjugation, various functional groups, and potential for biological and optical applications, was successfully obtained with high purity and yield using a conventional method. The title compound is a remarkable heteroaromatic compound with –ONNO-type tetradentate cage-like structure. On the other hand, its structure includes long alkyl chains attached to both the benzene ring and the imine moiety. The synthesized compound was analyzed by X-ray, FTIR, ¹H–¹³C NMR, and UV-Vis spectroscopies. The FTIR spectrum of the Schiff base is given in Fig. 2.

The synthesized Schiff base is aimed to contain many different functional groups and the most important groups to determine the formation of the desired structure are C=N, C–OH, and C=C. In this regard, when analyzing the spectrum of the compound, the vibrations observed in the range of 3050–2800 cm^{−1} correspond to aromatic and aliphatic C–H vibrations. Specifically, the aromatic C–H vibrations are observed at 3027 cm^{−1}, while the aliphatic C–H vibrations are observed between 2923–2852 cm^{−1}, consistent with existing literature [22]. The synthesized molecule has an –OH group close to the imine bond and high aromatic conjugation. In this case, the strong intermolecular H-bond can allow easy transfer of protons and observation of keto-enol transformation. For this reason, the –OH vibration was detected at a lower wavelength, appearing as a larger peak instead of a sharp peak, at about 2500 cm^{−1} [23]. Another important issue for the title compound is the formation of an imine bond. The imine vibration was identified at 1605 cm^{−1}, which is a lower wavelength compared to the carbonyl vibration of 2-hydroxy-4-octyloxy benzophenone at 1629 cm^{−1} [24]. On the other hand, C=C vibration peaks caused by

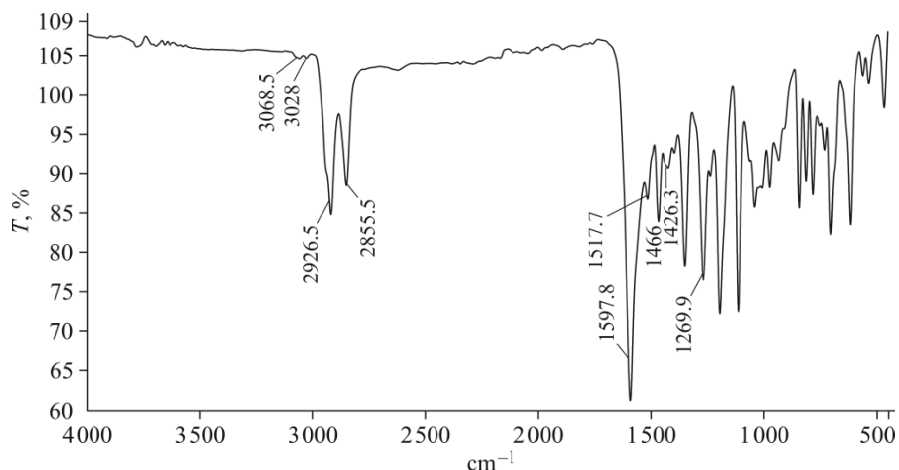


Fig. 2. FTIR spectrum of the Schiff base.

aromatic benzene rings were determined by the literature in the region between 1590-1515 cm^{-1} [25]. The peak at 1280 cm^{-1} is due to the C–O vibration of phenolic moiety [26].

The synthesized compound was also analyzed in different isotropic solvents because of determined electronic behaviors. The benzene moieties have π – π^* transitions and the peaks are expected at 230-270 nm. For the title compound, which has benzene rings with alkoxy moiety, the π – π^* transitions were detected at 212 nm in ethanol [27]. The most important transitions for the title compound are the n – π^* and π – π^* transitions of the imine group. At 300 nm and 383 nm, two strong peaks were detected in ethanol for π – π^* and n – π^* transitions, respectively [28]. In acetonitrile, the π – π^* transition was detected at a lower wavelength at 277 nm due to increasing stability of π orbital [29].

The title compound was analyzed by ^1H and ^{13}C NMR spectroscopies and the obtained spectra are given in Fig. 3. The spectra in DMSO have important chemical shifts according to electron density around the different types of atoms. For the synthesized compound in lower frequencies, aliphatic protons were seen as medium multiplet peaks in the range of 0.84-1.86 ppm (H46–H53). Another aliphatic protons attached to nitrogen and oxygen atoms were seen in 3.31 ppm and 3.91 ppm (H10–H14), respectively [30]. The synthesized compound has benzene rings with different functional groups, and aromatic protons were detected in the range 6.16-7.49 ppm (H1–H6, H19–H23) as different multiplet peaks consistent with the literature [31]. Another important peak for the synthesized compound is phenolic proton and the peak was seen as a singlet peak at 15.93 ppm. The mentioned -OH peak was detected at a high frequency due to the near imine group [32]. The ^{13}C NMR spectrum is also suitable for the designed molecule. The most important peak for the title compound is the imine peak and this peak was observed at 173.84 ppm [33]. The phenolic carbon was seen at 163.08 ppm [34]. The important carbons for the title compound were detected at 127.56-133.31 ppm (C1–C6, C19–C23); 67.93 (10,14) and 48.12 ppm (46) for the aromatic carbons, the aliphatic nitrogen-based and oxygen-based carbon atoms, respectively. Aromatic carbons were detected over a large area due to the attachment of different moieties [35, 36]. Another aliphatic CH_2 and CH_3 carbons in long alkyl chain peaks were detected at 14.40-31.67 ppm (C11–C13, C45–C53).

X-ray and optimized structure determinations. The molecular and optimized structures of the title compound are presented in Fig. 4 and 5, respectively. XRD analysis confirmed that the compound has an orthorhombic crystal system with *Pccn* space group. The unit cell parameters are: $a = 15.1474(5) \text{ \AA}$; $b = 26.6737(11) \text{ \AA}$; $c = 10.3762(4) \text{ \AA}$; $\alpha = \beta = \gamma = 90^\circ$; $V = 4192.4(3) \text{ \AA}^3$. Table 2 presents a comparison between the geometrical parameters calculated by DFT and the parameters obtained by XRD method. As a result of this comparison, the experimental parameters showed good agreement with the theoretical parameters.

O1–C16(1.348 $\text{\AA}$), C17–O2(1.442 $\text{\AA}$), C11–C4(1.470 $\text{\AA}$) and C3–N1(1.471 $\text{\AA}$) bonds form single bonds within the title compound. Similar results reported in other references are showing good agreement with the results of studied compound: (O1C6 = 1.3463(18) $\text{\AA}$ [37]; C2O5 = 1.361(4) $\text{\AA}$ [38]; C9O3 = 1.351(3) $\text{\AA}$ [39], (O2C16 = 1.424(3) $\text{\AA}$ [40];

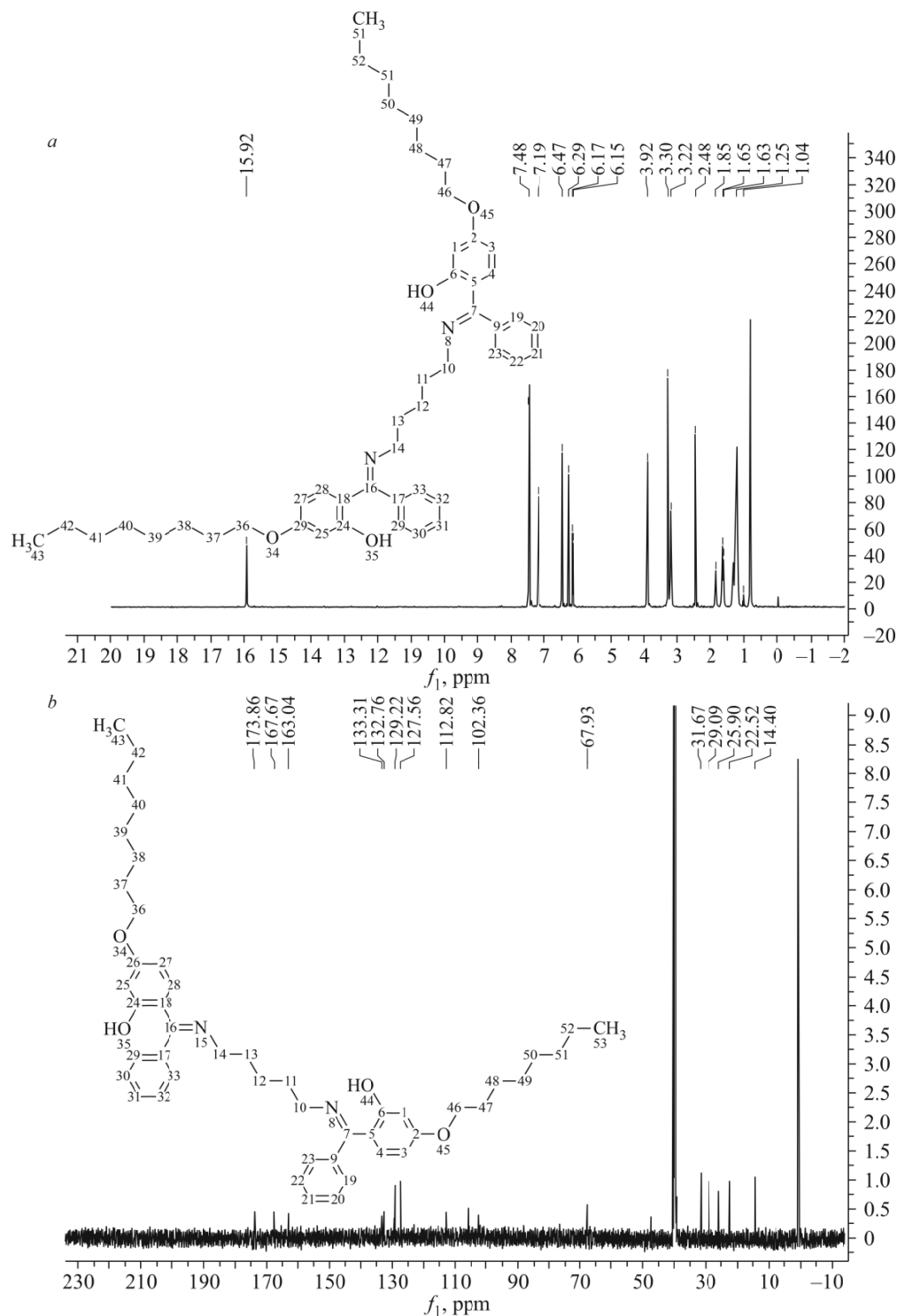


Fig. 3. ^1H – ^{13}C NMR spectra of the Schiff base.

$\text{O2C14} = 1.433(5) \text{ \AA}$ [41]; $\text{C5O4} = 1.406(5) \text{ \AA}$ [42], ($\text{C2C3} = 1.493(2) \text{ \AA}$ [43]; $\text{C2C21} = 1.457(3) \text{ \AA}$ [44]; $\text{C7C8} = 1.453(4) \text{ \AA}$ [45], ($\text{N2C22} = 1.459(4) \text{ \AA}$ [46]; $\text{N2C11} = 1.482(3) \text{ \AA}$ [47]; $\text{N1C8} = 1.470(3) \text{ \AA}$ [38]). Additionally, the bond distance of C4=N1 of the studied compound was obtained at $1.285 \text{ \AA}$ and well agreed with other studies: ($\text{N1=C7} = 1.282(6) \text{ \AA}$ [48]; $\text{C9=N1} = 1.267(5) \text{ \AA}$ [49]; $\text{N9=C8} = 1.273(5) \text{ \AA}$ [50]).

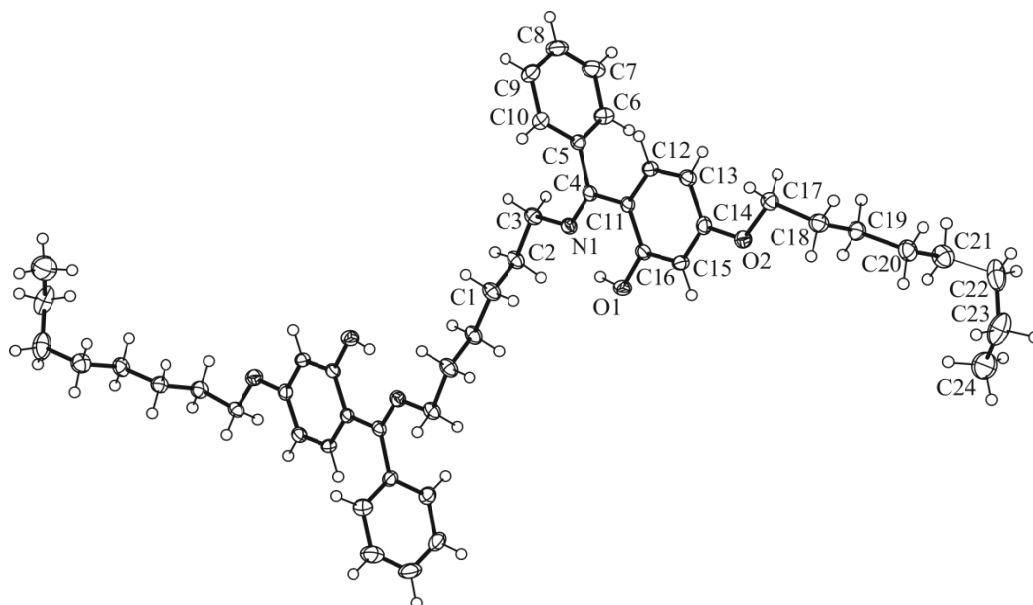


Fig. 4. Symmetrical molecular structure view by ORTEP-III.

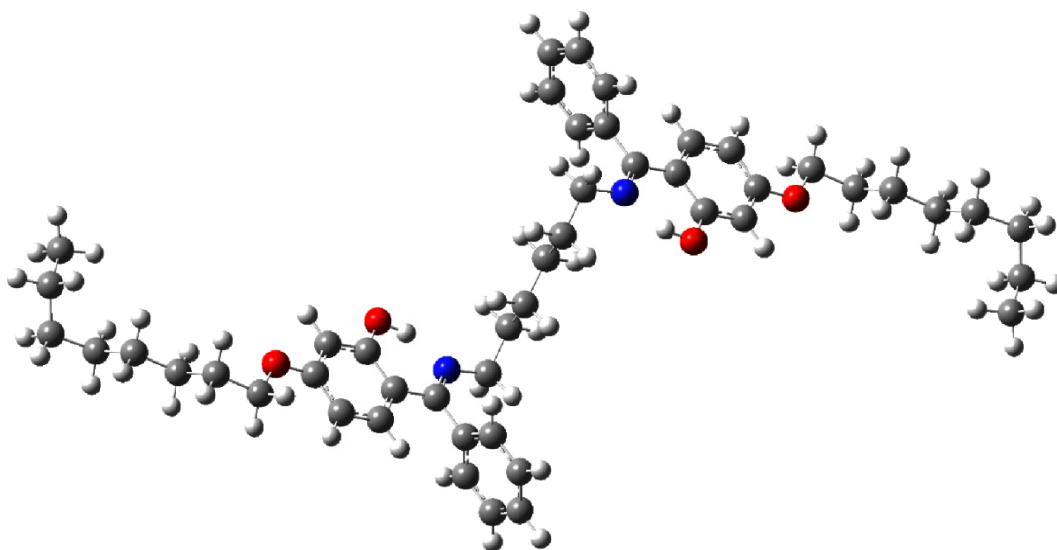


Fig. 5. Symmetrical optimized structure of the title compound.

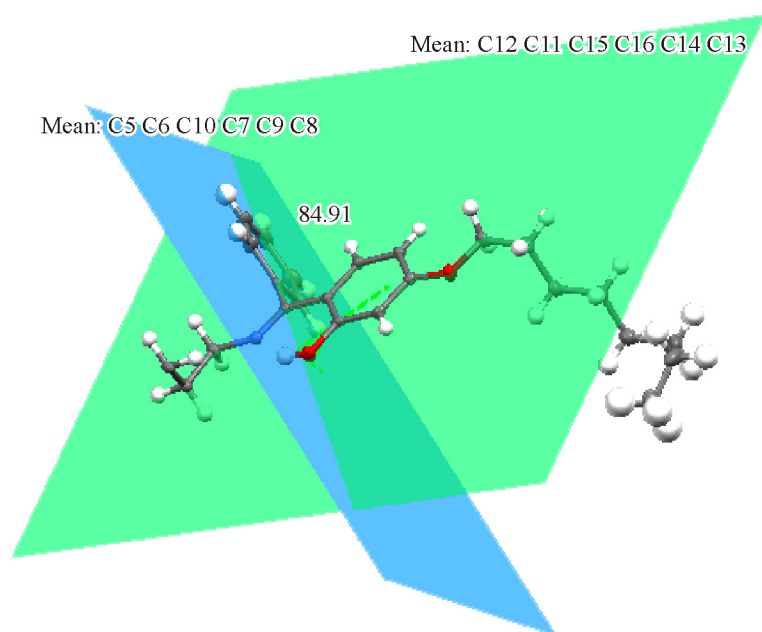
The dihedral angle formed by two phenyl rings (Ph1:C5/C10) and (Ph2:C11/C16) was calculated at 84.91° using Mercury program (Fig. 6). All possible hydrogen bond geometries are presented in Table 3. The stability of the compound structure relies significantly on these interactions. The Root Mean Square Deviation analysis (RMSD) was utilized for comparing X-ray and DFT structure's parameters. The RMSD value was calculated at $0.851 \text{ \AA}$, as presented in Fig. 7.

Hirshfeld surface (HS) analysis. HS analysis was conducted to validate the effects of various intermolecular interactions. This aids in recognizing the existence of hydrogen bonds and other weak intermolecular interactions within the crystalline structure. The molecular surfaces of Hirshfeld analysis were created using CrystalExplorer21 [51] by loading CIF format file of the crystal data obtained by X-ray. A normalized contact distance, denoted as d_{norm} , was utilized to produce HSs, depending on various factors, including d_i , d_e and Van der Waals radii. It can be calculated using the equation below:

$$d_{\text{norm}} = \frac{d_i - r_i^{\text{vdw}}}{r_i^{\text{vdw}}} + \frac{d_e - r_e^{\text{vdw}}}{r_e^{\text{vdw}}} \quad (1)$$

TABLE 2. Selected Optimized and Refined Parameters of the Compound

Geometrical Parameter	Experimental	B3LYP
Bond length, Å		
C4–N1	1.285	1.296
O1–C16	1.348	1.337
C17–O2	1.442	1.429
C11–C4	1.470	1.469
C3–N1	1.471	1.456
Bond angles, deg		
C17–O2–C14	117.11	119.22
C5–C4–C11	118.00	118.50
C11–C16–O1	121.14	121.81
C4–N1–C3	120.46	123.42
C9–C10–C5	124.23	120.39
Torsion angles, deg		
C13–C14–O2–C17	–1.8	0.5
C5–C4–C11–C12	5.1	3.2
C13–C14–O2–C17	–1.8	0.5
C4–C11–C16–O1	–2.1	–0.7
C3–N1–C4–C5	1.0	1.9

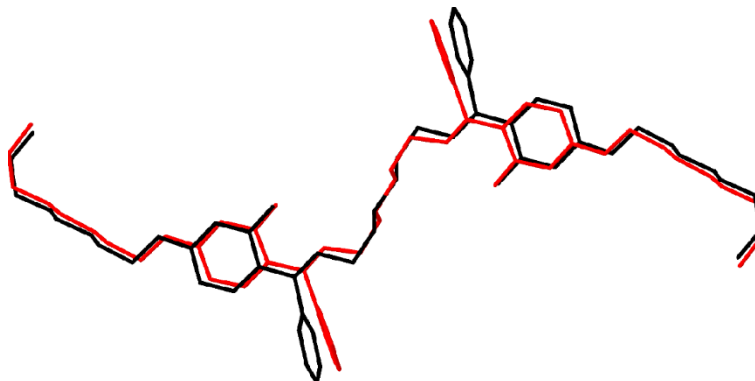
**Fig. 6.** The designated angle between two phenyl rings of the asymmetric structure.

The d_i (internal) and d_e (external) values represent the distances from the nuclei to the Hirshfeld surface concerning Van der Waals radii. 3D d_{norm} surfaces were visualized with various color-coded spots and areas, spanning from white to blue and red. The range of d_{norm} value extended from negative to positive values. The red regions indicate close contacts (with distances less than the sum of Van der Waals radii and negative d_{norm} values), white regions depict contacts with distances matching the sum of Van der Waals radii and d_{norm} values equal to zero, and blue areas indicate relatively longer intermolecular distances with positive d_{norm} values [52, 53].

TABLE 3. Distances (Å) and Angles (deg) of Hydrogen Bond

$D-H\cdots A$	$D-H$, Å	$H\cdots A$, Å	$D\cdots A$, Å	$D-H\cdots A$, deg
O1–H1C $\cdots$ N1	0.84	1.80	2.554	147.7
C1–H1B $\cdots$ N1	0.99	2.67	3.001	99.5
C6–H6 $\cdots$ O1 ^{#1}	0.95	2.57	3.441	151.5
C18–H18B $\cdots$ O2 ^{#2}	0.99	2.99	3.759	134.3
C21–H21A $\cdots$ O1 ^{#3}	0.99	2.93	3.915	169.2
C23–H23B $\cdots$ O2 ^{#4}	0.99	2.94	3.674	131.3

Symmetry codes: ^{#1} $-x+1, -y+1, -z+1$; ^{#2} $-x+1/2+1, y, z+1/2$; ^{#3} $x, y, z+1$; ^{#4} $x, -y+1/2+1, z+1/2$.

**Fig. 7.** The overlap between DFT and X-ray structures.

As seen from Fig. 8, the values of d_{norm} , d_e , d_i , shape index and curvedness range between -0.1030 to 1.3609 , 1.0732 to 2.4378 , 1.0737 to 2.5285 , -1 to 1 and -4 to 4 , respectively. Fingerprint plots in Fig. 9 show that the highest intermolecular interaction contributions of the compound are as follows: $H\cdots H$ (72.8%), $H\cdots C/C\cdots H$ (17.9%) and $O\cdots H/H\cdots O$ (7.6%). Fig. 10 displays Hirshfeld surface with red spots related to close contacts at the $C6'-H6'\cdots O1$ and $C6-H6\cdots O1'$ interactions.

Natural Bond Orbital Analysis. NBO analysis is a theoretical method used in computational chemistry to study the distribution of electrons in a molecule. It can be used to determine the transfer of charges between electron donors and electron acceptors, which is essential in understanding chemical bonding and reactivity. NBO analysis can also provide insights into hyperconjugative interactions, which involve the overlap of σ or π electrons between adjacent atoms, and it can help in studying non-covalent interactions, such as hydrogen bonding and Van der Waals interactions within a molecule [54]. NBO calculations were performed in NBO 7 suite [55] included in Gaussian '16 program package. The stabilization energy E^2 is assessed using the second-order perturbation method as provided here:

$$E^2 = q_i \frac{F^2(i, j)}{\varepsilon_j - \varepsilon_i}. \quad (2)$$

Here, q_i represents the occupancy of the donor orbital, ε_i and ε_j stand for diagonal elements (orbital energies) and $F(i, j)$ signifies the off-diagonal Fock matrix element. A high E^2 typically indicates a more intensive or stronger interaction between electron-donating and electron-accepting atoms. In other words, it indicates a stronger inclination of electron donors to transfer their electrons to electron acceptors and an enhanced degree of conjugation within the entire system.

Table 4 displays intermolecular hyperconjugative interactions involving π -electrons, such as the interaction from C16–C11 to N1–C4, C16–C11 to C12–C13, C15–C14 to C16–C11, C12–C13 to C15–C14, C5–C6 to C7–C8, C10–C9 to C5–C6, C7–C8 to C5–C6 and C7–C8 to C10–C9, with substantial energy contributions of 22.73 kcal/mol, 27.32 kcal/mol, 26.76 kcal/mol, 23.70 kcal/mol, 20.34 kcal/mol, 20.78 kcal/mol, 20.56 kcal/mol and 20.31 kcal/mol, respectively. Other interactions involve σ -electrons, including C12–C13 to O2–C14, C4–C11 to N1–C3, C16–C15 to O2–C14, C12–C11 to

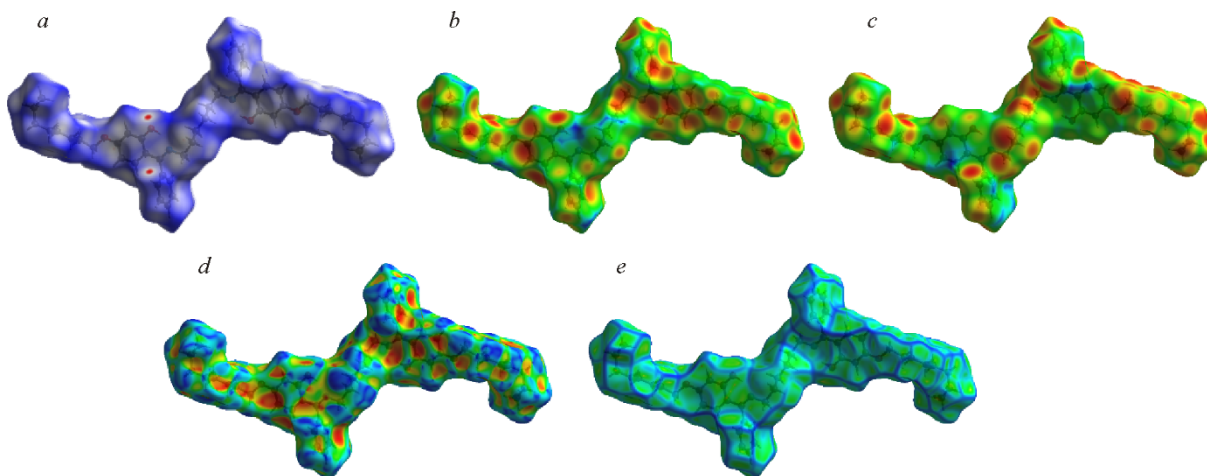


Fig. 8. 3D HS mapped with d_{norm} (a), d_c (b), d_i (c), shape index (d) and curvedness (e).

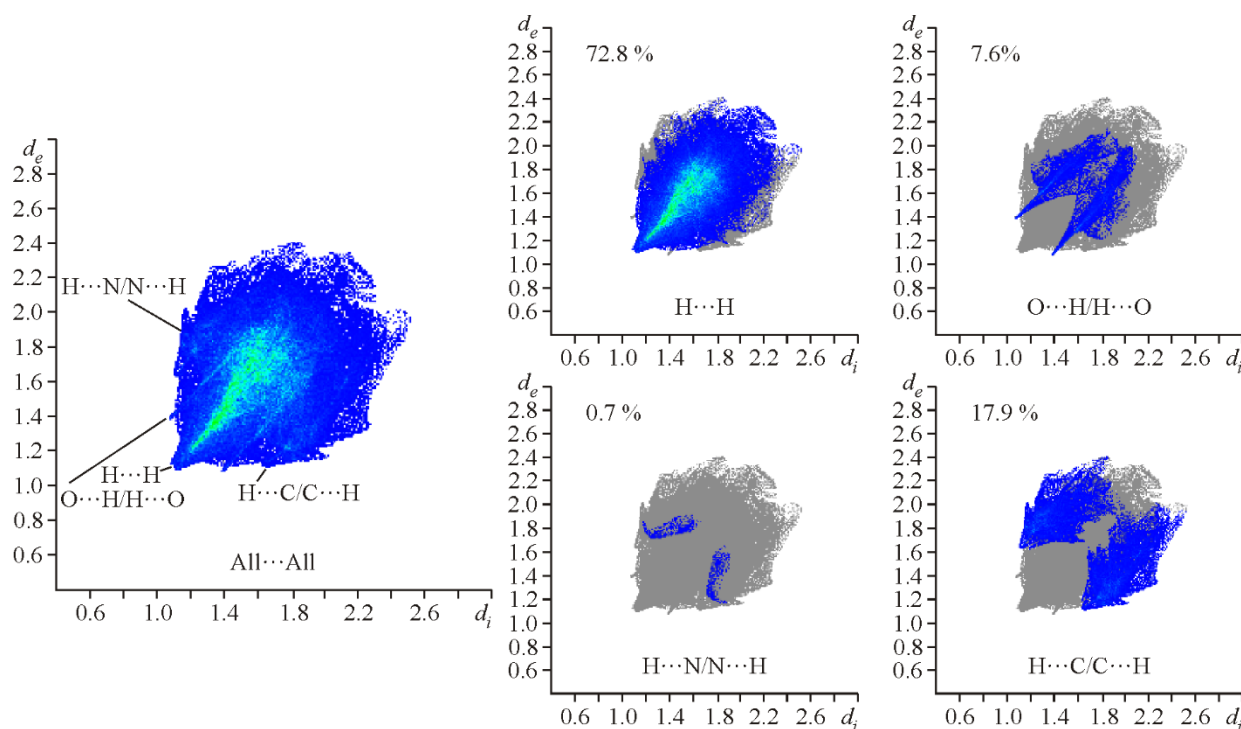


Fig. 9. 2D fingerprint plots visualizing the dominant intermolecular interactions.

O1–C16 and N1–C3 to C4–C11, with lower energy contributions of 4.76 kcal/mol, 4.92 kcal/mol, 3.52 kcal/mol, 3.42 kcal/mol and 4.08 kcal/mol, respectively. The lone pair electrons of O2 and O1 are contributed to the π -type antibonding orbital for C15–C14 and C16–C11, resulting in a stabilization energy of 29.98 kcal/mol and 40.59 kcal/mol. While the lone pair electrons of N1 are contributed to the σ -type antibonding orbital for C4–C5, resulting in a stabilization energy of 12.23 kcal/mol.

Frontier Molecular Orbitals. The E_{HOMO} and E_{LUMO} energies play a significant role in predicting chemical reactivity and stability in quantum chemistry. These energies are related to the ability of the molecule to gain or lose an electron in chemical and physical processes. A molecule with a higher energy HOMO orbital indicates the ability of the molecule to donate an electron to the low-lying unoccupied orbitals. On the other hand, the molecule with lower LUMO energy value exhibits a greater electron-accepting nature [56]. Fig. 11 shows the 3D shapes and the energy levels of the

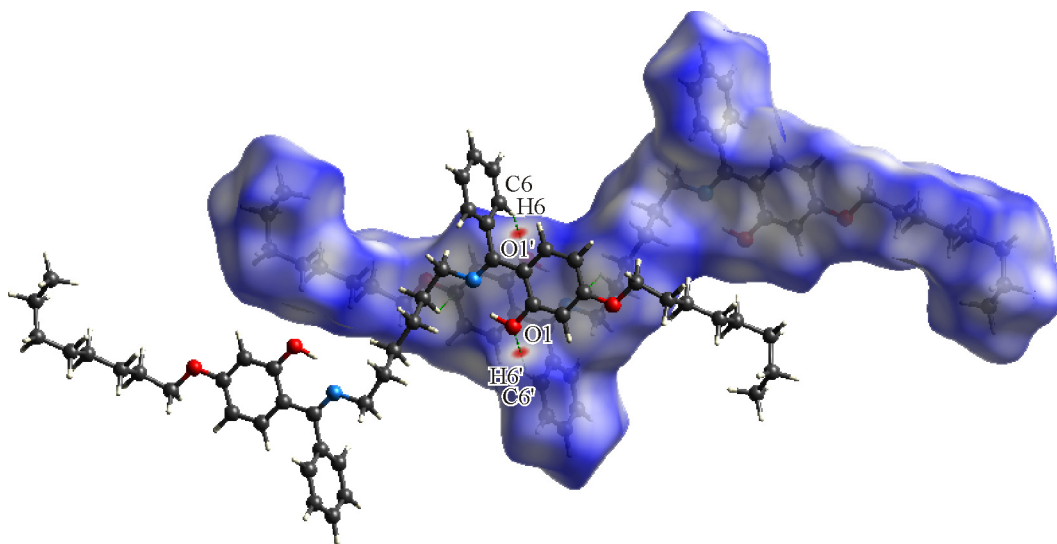


Fig. 10. View of 3D d_{norm} surface of the title molecule surrounded by adjacent molecules displaying close contacts.

TABLE 4. Selected Second-Order Perturbation Energies Associated with the $i \rightarrow j$ Electron Delocalization

Donor (<i>i</i>) (Occupancy)	Bond A–B	ED _A %, ED _B % ^{#1}	Acceptor (<i>j</i>) (Occupancy)	Bond A–B	ED _A %, ED _B %	E^2 ^{#2} , (kcal/mol)	$E_j - E_i$ ^{#3} , au	F_{ij} ^{#4} , au
1	2	3	4	5	6	7	8	9
BD N1-C4 (1.94363)	π	61.57, 38.43	BD* C16-C11 (0.48292)	π^*	60.05, 39.95	5.42	0.35	0.044
BD C16-C11 (1.56418)	π	39.95, 60.05	BD* N1-C4 (0.20179)	π^*	38.43, 61.57	22.73	0.26	0.073
BD C16-C11 (1.56418)	π	39.95, 60.05	BD* C12-C13 (0.34814)	π^*	55.80, 44.20	27.32	0.27	0.079
BD C15-C14 (1.66626)	π	56.13, 43.87	BD* C16-C11 (0.48292)	π^*	60.05, 39.95	26.76	0.28	0.080
BD C12-C13 (1.97505)	σ	49.97, 50.03	BD* O2-C14 (0.02775)	σ^*	32.37, 67.63	4.76	1.08	0.063
BD C12-C13 (1.73560)	π	44.20, 55.80	BD* C15-C14 (0.38945)	π^*	43.87, 56.13	23.70	0.28	0.076
BD C4-C11 (1.96764)	σ	49.70, 50.30	BD* N1-C3 (0.02397)	σ^*	39.15, 60.85	4.92	1.04	0.064
BD C5-C6 (1.65950)	π	50.97, 49.03	BD* C7-C8 (0.32853)	π^*	50.02, 49.98	20.34	0.28	0.068
BD C16-C15 (1.97493)	σ	50.19, 49.81	BD* O2-C14 (0.02775)	σ^*	32.37, 67.63	3.52	1.07	0.055
BD C10-C9 (1.66124)	π	50.03, 49.97	BD* C5-C6 (0.35297)	π^*	49.03, 50.97	20.78	0.28	0.069
BD C7-C8 (1.65766)	π	49.98, 50.02	BD* C5-C6 (0.35297)	π^*	49.03, 50.97	20.56	0.28	0.068
BD C7-C8 (1.65766)	π	49.98, 50.02	BD* C10-C9 (0.32432)	π^*	49.97, 50.03	20.31	0.28	0.068
BD C12-C11 (1.97237)	σ	48.86, 51.14	BD* O1-C16 (0.01830)	σ^*	34.01, 65.99	3.42	1.10	0.055

TABLE 4. (Cont.)

1	2	3	4	5	6	7	8	9
BD N1-C3 (1.98465)	σ	60.85, 39.15	BD* C4-C11 (0.03547)	σ^*	50.30, 49.70	4.08	1.20	0.063
LP O2 (1.83254)	π	—	BD* C15-C14 (0.38945)	π^*	43.87, 56.13	29.98	0.34	0.096
LP O1 (1.79881)	π	—	BD* C16-C11 (0.48292)	π^*	60.05, 39.95	40.59	0.31	0.108
LP N1 (1.83729)	σ	—	BD* C4-C5 (0.04651)	σ^*	51.07, 48.93	12.23	0.78	0.090

^{#1}The percentage electron density of atom A and atom B. ^{#2}The energy of hyperconjugative interaction (stabilization energy). ^{#3}The energy difference between donor and acceptor. ^{#4}The Fock matrix element.

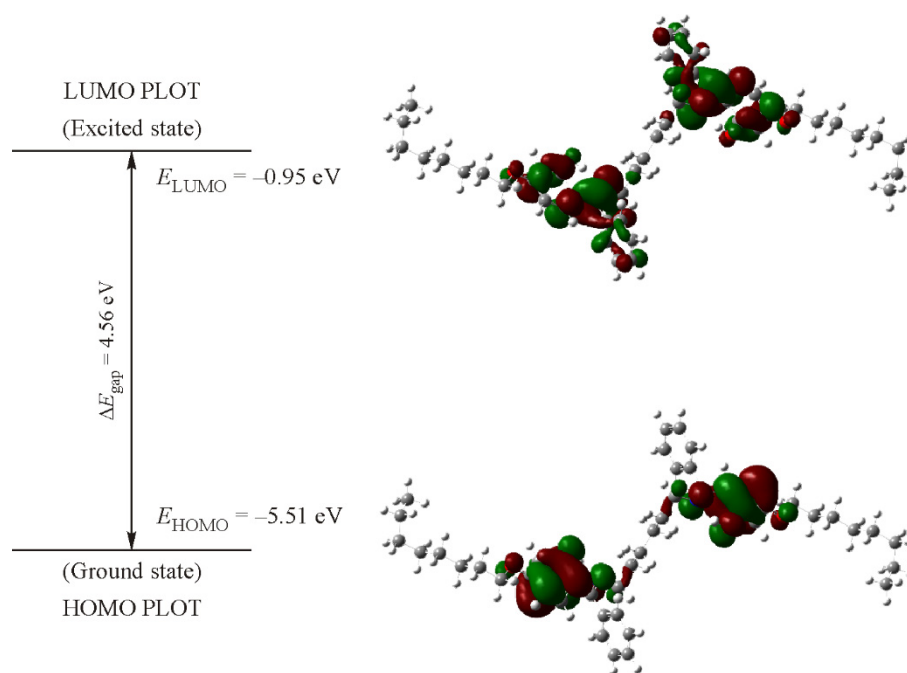


Fig. 11. The surface maps of the HOMO and LUMO frontier orbitals computed at B3LYP/6-31G(*d,p*) level.

HOMO and LUMO frontier orbitals. The red and green colours represent the positive and negative phases of the orbitals respectively.

The LUMO orbital is localized in the imine group and oxygen atoms while the HOMO is localized in the imine group and oxyphenol group. The HOMO orbitals (HOMO, HOMO-1, HOMO-2) exhibit energy levels of -5.5192 eV, -5.5337 eV, and -5.8760 eV, respectively, whereas the LUMO orbitals (LUMO, LUMO+1, LUMO+2) have the energies of -0.9572 eV, -0.9447 eV, and -0.2985 eV, respectively. HOMO-LUMO energy gap with large value (4.562 eV) implies a molecule with low polarity and reduced chemical reactivity. Conversely, a small energy gap suggests a diminished kinetic stability but an enhanced chemical reactivity and polarizability, as illustrated in Table 5.

Electrostatic potential (ESP). Symmetrical nature of the molecule allows us to investigate one half of the molecule in terms of the ESP partial atomic charges. The positively charged regions of the neutral molecule are predicted to be the alkyl (R) tail and slightly the phenyl group. The negative charge is localized mostly on the oxygen atom of the R–O group along with the nitrogen atom. It is suitable to consider the molecule in terms of its functional units such as R–O group, phenyl

TABLE 5. Some Calculated DFT Descriptors

Parameter	Values
E_{HOMO} , eV	−5.5192
E_{LUMO} , eV	−0.9572
Ionization potential I , eV	5.5192
Electron affinity A , eV	0.9572
Energy gap E_g , eV	4.5620
Electronegativity χ , eV	3.2382
Chemical potential μ , eV	−3.2382
Chemical hardness η , eV	2.281
Chemical softness s , eV ^{−1}	0.219
Electrophilicity index ω	2.298

(Ph) group, phenol (Ph–OH) group and the =N–R unit in the mid region to investigate the electron attachment and ionization processes. For this purpose, the total ESP partial charges are summarized in Table 6.

In terms of the changes in the total partial atomic charges of molecular units, the present molecule tends to be ionized from phenol and =N–R groups while the change in the total charges localized on –Ph and R–O groups is found insignificant. In contrast to this, in an electron attachment process, the molecule tends to be transformed into anionic form over its –Ph group.

Molecular electrostatic potential analysis. Molecular electrostatic potential (MEP) is employed to get further information about the reactive sites of the molecule. The MEP was computed by using B3LYP hybrid functional in 6-31G(*d,p*) basis to predict the sites of electrophilic and nucleophilic reactions [57]. MEP map readily reveals regions characterized by varying electron densities, ranging from high to low. The red color indicates the presence of the most negatively charged region, suggesting susceptibility to electrophilic attacks at that site. Conversely, the blue color designates the region with the highest positive charge localized in a suitable region of the molecule, indicating its potential for nucleophilic attacks. Meanwhile, the green color represents a zero potential region [58]. In Fig. 12, electronegative atoms like O1 and O2 are enclosed by red and yellow regions, indicating electron-rich areas and suggesting them as potential active sites for positively charged ions (electrophilic attack). In contrast, hydrogen atoms are surrounded by blue regions, indicating suitable sites for nucleophilic attack.

Electrophilicity-based charge transfer method with DNA bases. Electrophilicity-based charge transfer (ECT) analysis is a valuable study for examining the behaviour of molecules and DNA bases as either electron donors (nucleophilic) or electron acceptors (electrophilic). Furthermore, it helps specify the direction of charge transfer between DNA bases and the present molecule. In this context, two situations can be explored: When $ECT > 0$, it signifies the movement of charges from the DNA base to the functional group, while $ECT < 0$ indicates the transfer of charges from the functional group to the DNA base [59].

The electron affinity (EA) and ionization potential (IP) were determined based on the energies of neutral (N), anionic (N[−]), and cationic (N⁺) species using the following equations:

$$IP = [E(N-1) - E(N)], \quad (3)$$

TABLE 6. The Total ESP Charges of Molecular Units

Molecular unit	R–O group	Phenol group	–Ph group	=N–R group
Neutral	−0.10	+0.01	+0.15	−0.31
Cation	−0.04	+0.33	+0.17	−0.22
Anion	−0.18	−0.08	−0.06	−0.38

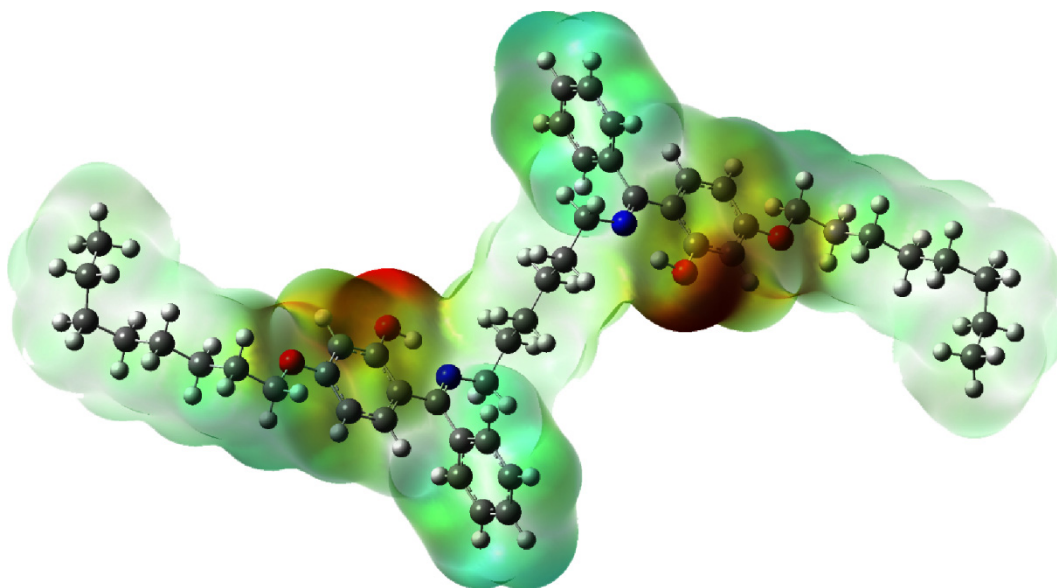


Fig. 12. MEP map of the title compound.

$$EA = [E(N) - E(N + 1)]. \quad (4)$$

In this study, two different molecules were taken into account, where molecule A represents the studied molecule and molecule B represents one of the DNA bases (adenine, cytosine, thymine, or guanine). The direction of charge transfer depends on the ECT value. If it is greater than zero, the charge will flow from B to A. On the other hand, if it is less than zero, the charge will move from A to B. The calculation of ECT was based on the following equations:

$$(\Delta N_{\max})_A = \mu_A / \eta_A, \quad (5)$$

$$(\Delta N_{\max})_B = \mu_B / \eta_B, \quad (6)$$

$$ECT = (\Delta N_{\max})_A - (\Delta N_{\max})_B. \quad (7)$$

Based on the information provided in Table 7, the ECT values for the DNA bases (adenine, guanine, cytosine, and thymine) are as follows: 1.813, 1.872, 1.890, and 1.971, respectively. This indicates that the DNA bases exhibit nucleophilic characteristics by donating electrons. Conversely, the studied molecule is an electron acceptor with electrophilic nature.

Effects of Schiff base on LCS. DACI is a cationic surfactant containing a ten-carbon apolar alkyl chain and a polar head. The surfactant in question was used as the key component to form micelles and KCl was used as a salt to determine micelle type and stability. DACI/KCl/H₂O system was used to obtain isotrope and nematic phase and also S-(-)-Limonene was used as an optically active molecule to helical order for the cholesteric phase. In this respect, a cholesteric lyotropic phase with a helical pitch of 240 μm was created by the DACI/KCl/H₂O/S-(-)-Limonene system [21, 60]. The Schiff base solution in S-(-)-Limonene was added to the cholesteric system. The resulting phase changes were determined based on the texture observed in POM images to assess the effect of the Schiff base at a range of concentrations from $7.00 \cdot 10^{-5}$ M to $2.25 \cdot 10^{-3}$ M, depending on the solubility of the Schiff base. At lower concentrations, as the viscosity increased, the helical structure was

TABLE 7. Calculated ECT Values Using the DFT Method

Compound & DNA bases	IP, eV	EA, eV	M , eV	H , eV	$\Delta N_{\max}$
Title compound	6.487	0.180	-3.333	3.154	-1.057
Adenine ECT = 1.813	7.778	-1.358	-3.210	4.568	-0.703
Guanine ECT = 1.872	7.293	-0.989	-3.152	4.141	-0.761
Cytosine ECT = 1.890	8.235	-1.020	-3.607	4.628	-0.779
Thymine ECT = 1.971	8.950	-0.670	-4.140	4.810	-0.861

disrupted and a conical texture expressing the hexagonal structure was observed [12, 61]. The $7.00 \cdot 10^{-5}$ M Schiff base was added, the conical texture was observed due to the hexagonal phase (Fig. 13). In the $2.80 \cdot 10^{-4}$ M Schiff base added, the nematic phase transition was started and in upper concentration, the nematic texture was detected. The results show that the synthesized Schiff base is suitable for lyotropic media as it ensures that the micelles continue to be arranged, that is, the liquid crystal properties continue in the studied concentration range. As increasing concentration of Schiff base, an increasing amount of settle on or in micelles is provided to micelles lower order. On the other hand, the order of micelles was protected in one direction, and result of this attraction nematic phase texture was seen on POM and a homogenous anisotropic solution remained because of the suitability of Schiff base with polar and apolar moieties.

It is well known in the literature that the surface active agents, commonly known as surfactants can form several self-aggregated structures namely micelles, reverse micelles, and liquid crystalline phases in aqueous solutions that can generate hydrophobic domains to solvate and solubilize the non-polar species. In the specified conditions, the development of spectroscopic properties may be achieved due to the attraction between guest-host bio-attractive molecules and anisotropic media. The different and controllable molecular order of phase type is an important biomimetic control factor for water-based systems. The lyotropic liquid crystal media has an important optical advantage due to order orientation and in this respect we analyzed the DACI/KCl/H₂O/S(-)-Limonene and DACI/KCl/H₂O/S(-)-Limonene/Schiff base systems by UV-Vis. spectroscopy to determine the evolution of the lyotropic system with the addition of Schiff base. For this purpose, we analyzed isotrope, nematic and cholesteric phases with DACI/KCl/H₂O/S(-)-Limonene. The spectrum of the mentioned system without Schiff base is given in Fig. 14.

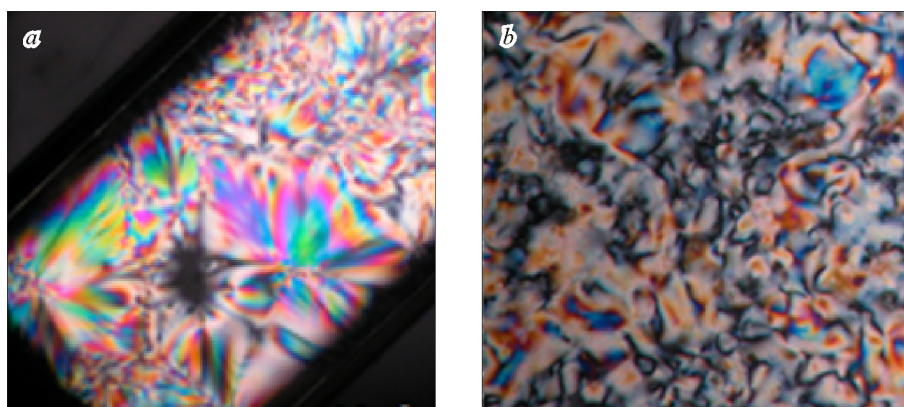


Fig. 13. Hexagonal (a) and nematic (b) phase texture.

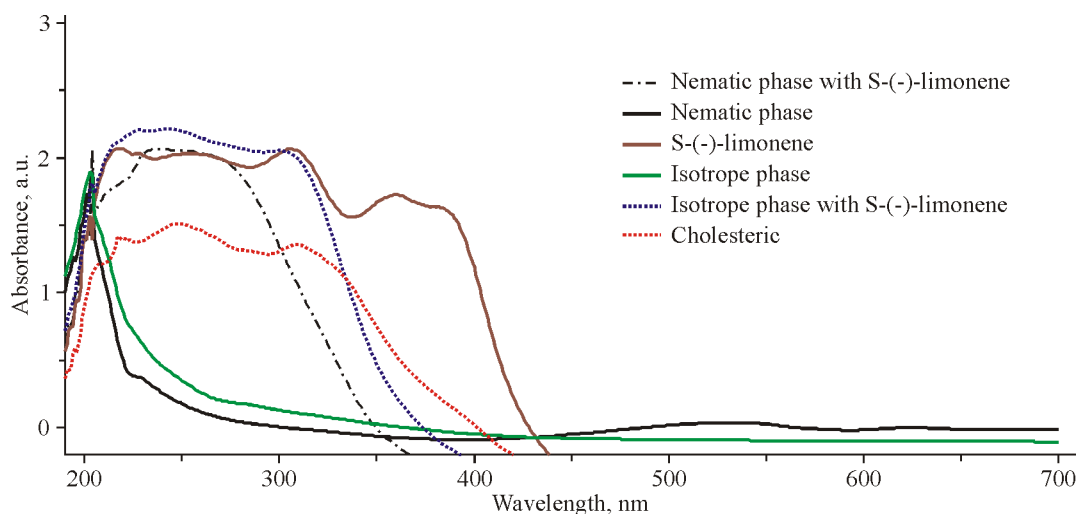


Fig. 14. The spectrum of DACI/KCl/H₂O/S(-)-Limonene system without Schiff base at 25 °C (see the electronic version).

The isotrope phase without S-(-)-Limonene has electronic transitions in the lower wavelength area and the nematic phase without optically active molecule has a different transition from the isotrope phase about 500-600 nm. The observed situation is thought to be due to orientation in the interaction of light and micelles. A guest molecule can transfer optical properties to the host system, and in this study, primarily S-(-)-Limonene transferred the chirality to micelles and changed the micelle surface causing a shift in electronic transitions. Upon adding S-(-)-Limonene to all phases, cholesteric, nematic and isotrope phases, the electronic transitions of S-(-)-Limonene were seen as dominant. On the other hand in all phases, the electronic transitions of S-(-)-Limonene were recorded a shift to lower wavelength. The determined blue shift may be the reason settle of the chiral molecule in micelle and aggregation of micelles [62].

The spectrum of the mentioned systems containing Schiff base at 25 °C is given in Fig. 15. In the spectra of systems containing Schiff base as a guest molecule, it has been observed that the electronic transitions located at high wavelengths belonging to Schiff base, and disappeared in the isotropic, nematic and cholesteric phases. In the isotrope phase, a significant blue shift was determined in Schiff base electronic transitions. On the other hand by looking at the DACl/KCl/H₂O/S-(-)-Limonene system, a small red shift was detected due to the changing of the micelle environment and molecular attractions. In the nematic phase, electronic transitions of Schiff base exhibited similar behavior within the isotrope phase by significant blue shift. On the other hand, in the nematic phase, electronic transitions of the Schiff base have a superior redshift according to the isotrope phase. In the cholesteric phase, the Schiff base electronic transitions displayed a similar blue shift with isotrope and nematic phase but the cholesteric system demonstrated a slight red shift and a distinct hyperchromic shift compared to the other phases [63, 64].

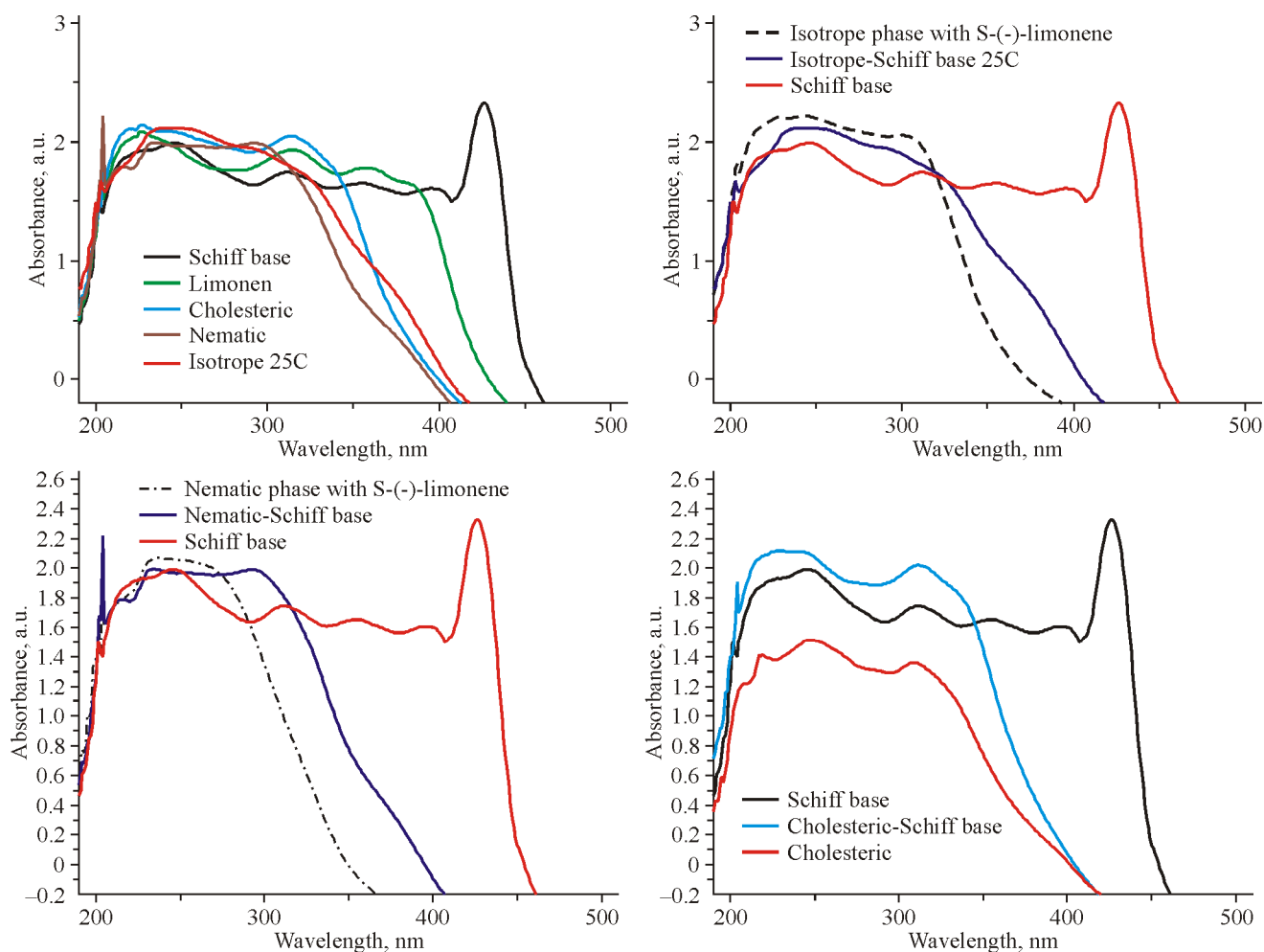


Fig. 15. The spectrum of DACl/KCl/H₂O/S-(-)-Limonene system with Schiff base at 25 °C.

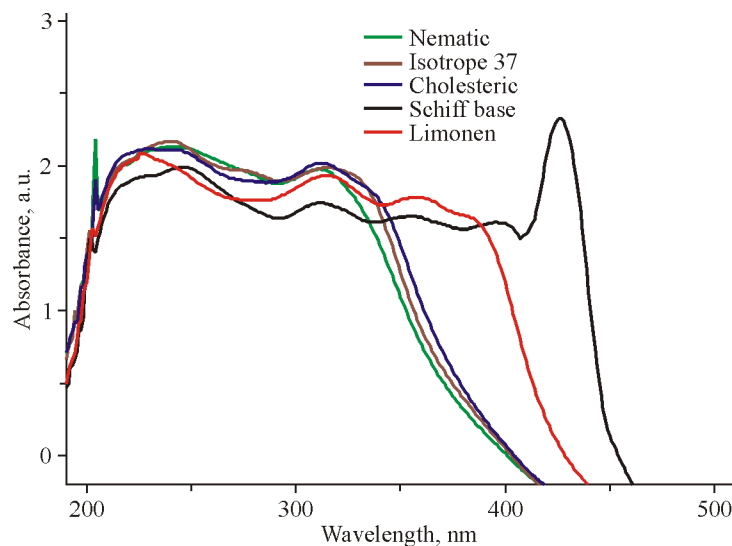


Fig. 16. The spectrum of DACI/KCl/H₂O/S-(-)-Limonene system with Schiff base at 37 °C (see the electronic version).

The spectrum of the mentioned system containing Schiff base at 37 °C is given in Fig. 16. Temperature is also an important factor for lyotropic liquid crystals due to changes in some properties such as orientation and fluidity. Consequently, all prepared phases researched at 37 °C are important for living organisms. The prepared system showed similar spectroscopic properties at 37 °C and anisotropic properties kept on without change. In light of all these results, the synthesized Schiff base is a suitable and important molecule with a symmetric structure, polar-apolar functional groups and potential biological properties for lyotropic crystal media.

CONCLUSIONS

A new tetra-dentate ONNO type Schiff base was synthesized and characterized using several spectroscopic methods. The information on single crystal structure was obtained using the X-ray diffraction method. The DFT calculations were determined using Gaussian 16 on a supercomputer cluster. The geometrical parameters of the title compound were calculated using DFT at B3LYP method and showed good agreement with experimental results. Several studies have been analyzed theoretically using the DFT approach which cannot be done through experimental methods. Hirshfeld analysis showed that red spots on the surface are related to close contacts and found at the C6' $\cdots$ H6' $\cdots$ O1 and C6 $\cdots$ H6 $\cdots$ O1' interactions. The high energy gap (4.48 eV) between HOMO–LUMO levels indicates that the title compound reveals low polarity and reduced chemical reactivity. MEP map presents that the potential active sites for positively charged ions are around O1 and O2 atoms with electrophilic attack while hydrogen atoms are indicating suitable sites for nucleophilic attack. Due to the analysis performed using ECT, DNA bases represent electron donors while the studied molecule represents electron acceptors.

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CONFLICT OF INTERESTS

The authors of this work declare that they have no conflicts of interest.

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