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B– Theoretical Sciences

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B– Teorik Bilimler

Volume/Cilt 10 Number/Sayı 2 – August / Ağustos 2022

ESKİŞEHİR TECHNICAL UNIVERSITY JOURNAL OF SCIENCE AND TECHNOLOGY
B- Theoretical Sciences
Eskişehir Teknik Üniversitesi Bilim ve Teknoloji Dergisi B – Teorik Bilimler

Volume: 10 / Number: 2 – August / 2022

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RESEACRH ARTICLE

SYNTHESIS, CHARACTERIZATION AND THEORETICAL CALCULATION OF *4-(((1H-IMIDAZOL-2-YL)METHYLENE)AMINO)PHENOL*

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ABSTRACT

In this study, the Schiff base 4-(((1H-imidazole-2-yl)methylene)amino)phenol (3), has been synthesized and the structure of the compound was characterized by elemental analysis, FTIR, ^{1}H NMR, ^{13}C NMR, and UV-Vis spectroscopic techniques. The correlation between theoretical and experimental spectroscopy data was examined. The acidity constant was calculated by using the PM6 method in the MOPAC2012 program and the DFT method in Gaussian09 program at B3LYP/6-311+G(d,p) levels at gas and liquid phases at 25 °C. After deciding the stable conformation of the synthesized molecule, HOMO, LUMO, MEP, and SAS theory were calculated using the B3LYP / 6-311+g(d, p) level.

Keywords: Schiff Base, DFT, Theoretical Calculation, Stable conformation, pKa

1. INTRODUCTION

Schiff bases, N-substituted imine derivatives, are not only used in organic chemistry but also as ligands [1-3]. The first preparation of Schiff bases was reported in 1864 by H. Schiff [4]. Since then, various methods for the synthesis of Schiff bases have been described [5]. The simple imine derivatives are generally synthesized from the condensation of aldehyde and primary amines. Because Schiff base chemistry has organic, inorganic, organometallic, and complex (Bidentate, Tridentate, Tetradentate, and Polydentate Schiff's bases according to the bonds they make with the metal applications) it has found many common uses in polymer and drug chemistry [6-10]. It is known that Schiff bases, which have biological activity, have antibacterial and antitumor properties depending on their electron attracting or electron-donating groups [11-13].

In the literature, there is no information on the acidity constant of the molecule in this study. There is a close interest between the acidity constant and the structure, properties, tautomeric state, formation, and reaction of the substance. There are various methods for determining the acidity constants such as potentiometric titration, spectrophotometric determination, and conductivity. The Ultraviolet-Visible spectrophotometric method is the most widely used and most sensitive method among other methods for the determination of acidity constants. Although this method takes a lot of time, it is preferred because it requires few substances and is very sensitive [14]. Theoretical calculations are economical methods that can be applied without chemical consumption, where laboratory conditions can be adjusted. Due to its practicality and speed, theoretical studies have found many application areas.

In this study, the synthesis (Scheme 1) characterization of 3 substances, which are thought to have active drug properties, was synthesized by the method of obtaining similar compounds, although the same substance is not found in the literature. [15, 16]. The characterization of the synthesized structure was carried out and spectroscopic studies were supported by the DFT calculation method. To find the

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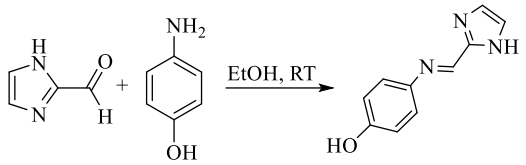
acidity constant, the sum of the electronic and thermal Free Energy of the Schiff base was calculated using the DFT method in gas and aqueous medium at room temperature. The pKa of the molecule was calculated from the sum of the electronic and thermal Free Energy. Calculations were made in Gaussian09 program with the DFT method at B3LYP/6-311G(d,p) level and MOPAC2016.



(1) **(2)** **(3)**

Scheme 1. Synthesis of 4-(((1H-imidazole-2-yl)methylene)amino)phenol **(3)**.

2. EXPERIMENTAL SECTION

2.1. General Procedures

Melting points were taken with the Mettler-Toledo MP90 device. Infrared spectra were recorded in the range of 4000-400 cm^{-1} on a Perkin Elmer precisely Spectrum 100 FT-IR spectrometer using KBr disks for solid samples. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on an Aligent 400 MHz DD2 spectrometer operating at 400.13 MHz for proton and at 100.62 MHz for carbon. ^{1}H NMR spectra were measured for ca. 25-30% solutions in DMSO-d_6 unless otherwise indicated and all chemical shifts are expressed relative to TMS (Me_4Si). Analytical thin-layer chromatography was carried out using aluminum-backed plates coated with Merck Kieselgel 60 GF254. UV-vis spectra were recorded with SHIMADZU UV-3150 UV-Visible spectrophotometer.

2.2. Synthesis

1H-imidazole-2-carbaldehyde (1 mmol) was dissolved in absolute ethanol (50 mL) and the temperature was raised to 60°C and stirring was continued at this temperature until the aldehyde dissolved [5]. Then 4-aminophenol (1 mmol) was added to the mixture. The entire mixture was stirred at room temperature and the progress of the reaction was monitored by TLC. The reaction mixture was poured onto crushed ice until a colored solid phase was formed. The separated solid product was filtered and recrystallized with ethanol.

2.2.1. ***4-(((1H-imidazol-2-yl)methylene)amino)phenol (3)*****:** This compound was obtained as brown powder (72%), mp 223 ºC; Anal. Calcd. for $C_{10}H_9N_3O$: C, 64.16; H, 4.85; N, 22.45; O, 8.55. Found: C, 63.30; H, 5.16; N, 21.61; O, 9.36. FT-IR (KBr, disk, ν cm-1): 3280 (O-H, N-H peak overlapped with O-H peak and remained below O-H peak), 3144-3069 (C-H, aromatic), 1621 (C=N), 1581-1444 (C=C, aromatic), 1247 (C-O) ^{1}H NMR (400 MHz, DMSO-d6) δ 12.93 (s, 1H phenol OH), 9.57 (s, 1H imidazole NH), 8.40 (s, 1H imine C=N), 7.22 (dd, J = 33.6, 24.9 Hz, 4H benzene), 6.80 (d, J = 8.7 Hz, 2H imidazole). ^{13}C NMR (101 MHz, DMSO-d_6) δ 156.90 (s), 147.66 (s), 145.71 (s), 142.36 (s), 130.83 (s), 122.89 (s), 120.14 (s), 116.23 (s).

3. THEORETICAL CALCULATIONS

3. 1. General Method

In the calculations for the molecule by using Intel(R) Core(TM) i5 X 3230M, 2.60 GHz, K55VD.411, 988B RPGA socket, X16 chipset workstation, (Marvin Beans, 2010 https://chemaxon.com/products/marvin) programs and CS ChemOffice Pro 12.0 for Microsoft Windows (CS ChemOffice Pro) and Gaussian 09 (Gaussian 09, 2009) program [17-20] the following calculation methods are used: Calculations with Gaussian 09 program were done with the DFT method, B3LYP

function and 6-311+g(d,p) basis set. In order to determine the most stable conformations of molecules, after drawing the molecules in the ChemDraw program, their stable conformations were calculated by transferring them to Marvin Beans (Marvin Beans, 2010 https://chemaxon.com/products/marvin)program. The calculated stable conformations of the molecule are minimized in the Chem3D program. The most stable conformations were calculated again by optimizing the molecule that was minimized in the Gaussian09 program with the "opt = mod redundant B3LYP/6-311+G(d,p)" in the DFT method. Thermodynamic results from the most stable conformations of molecule calculated were calculated with “freq B3LYP/6-311+G(d,p)”.

The compound has been investigated with the Gaussian09 program by DFT method B3LYP/6-311+G(d,p) in vacuum and water phases. The UV-Vis spectra of the stable forms of the compounds have been determined and their electronic transition properties, the shifts depending on the solvents and the HOMO-LUMO (Highest Occupied Molecular Orbital- Lowest Unoccupied Molecular Orbital) values, Molecular Electrostatic Potentials (MEP) and Solvent Accessibility Surface (SAS) have been calculated.

3.2. Theoretical Calculation of pK_a

3.2.1. DFT method

The studied molecules were drawn with the ChemDraw Professional program [18] and the optimization of the molecules was performed with the Gaussian program [19]. Secondly, input files of molecules have been established in GaussView5 software [20]. In the last step, input files were created by using the B3LYP/6-311+G(d,p) [21-26] level of theory and transferred to the Gaussian09W packet program [19, 27] for calculation.

The acidity constants are directly related to the free energy of the deprotonation Reaction Equation 1.

$$AH \rightleftharpoons A^- + H^+ \quad (1)$$

and defined as given in Equation 2.

$$pK_a = \Delta G_R / 2.303\ RT \quad (2)$$

The deprotonation of a compound in an aqueous solution can be represented as a part of a thermodynamic cycle (Figure 1). Figure 1 explains the interrelationship between the gas and solution thermodynamic parameters [28, 29].

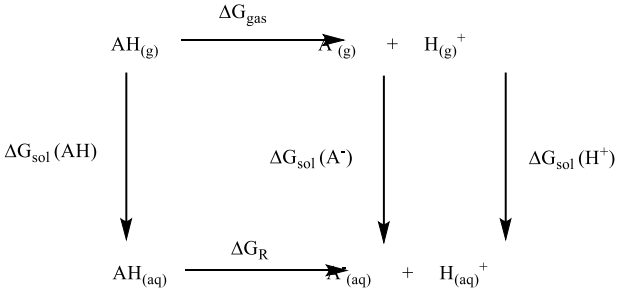


Figure 1. The interrelationship between the gas phase and solution thermodynamic parameters

One part of this cycle, ΔG_{gas} is the gas-phase deprotonation energy of the molecule. Three other parts ΔG_{sol} (AH), ΔG_{sol} (A^-), ΔG_{sol} (H^+) are the free energy of solvation of the protonated and deprotonated form of the molecule and the proton, respectively. The last part of the cycle ΔG_R,is the Sum of electronic and thermal Free Energies of deprotonation in solution and can be calculated as given in Equation 3.

$$\Delta G^o_{aq} = [\Delta G^o_s (A-) + \Delta G^o_s (H+) - \Delta G^o_s (AH)] + [\Delta G^o_g(A-) + \Delta G^o_g(H+) - \Delta G^o_g(AH)] \quad (3)$$

The total energies are given in Hartree's using the conversation factor 1 Hartree =627.5095 kcal mol^{-1}. The value of $\Delta G_{sol}(H^+)$ was taken as -48216.98 kcal mol^{-1} and $\Delta G_g(H^+)$ was taken as -48140.08 [30].

3.2.2. MOPAC method

For pKa calculation with Mopac program, MOPAC2016, Version: 17,039W was used. Since this program only calculates the pKa of hydroxyl hydrogens, the pKa value of the phenolic hydrogen (O-H) in the compound was calculated. In the calculation, the keywords "pm6 example of normal geometry definition debug ef charge=0", "oldgeo pm6 example of normal geometry definition debug ef charge=0", and "oldgeo pm6 gnorm=0.05 precise sparkle bfgs xyz pka let charge=0" used. Calculated pKa results are given in Table 7. http://openmopac.net/manual/pka.html

3.2.3. MarvinSketch method

Calculation of pKa with the MarvinSketch program was made using the version of MarvinSketch 20.6 (Marvin Beans, 2010 https://chemaxon.com/products/marvin). With this program, pKa values of nitrogen in the imidazole ring (CH = N), nitrogen in the imine group (CH = N), nitrogen-bound hydrogen in the imidazole ring (N-H), and oxygen-bound hydrogen in the phenol structure (O-H) were calculated. In the calculation, Mode: macro, Acid / base prefix: dynamic, Min basic pKa: -2, Max acidic pKa: 16 and Temperatura (K): 298 were selected [31]. The stacked pKa results are given in Table 7.

4. RESULTS AND DISCUSSION

4.1. Spectroscopic Results

4.1.1. UV-Vis spectroscopy

The UV spectrum of the studied molecule was taken between 190nm and 400nm in ethanol at room temperature as in the literature [32] (Figure 2). Generally, in the electronic absorption spectra of Schiff base compounds exhibit strong absorption bands at 266 nm. The band observed at 266 nm is the band belonging to the π-π * transition, which the band belonging to the n-π * transition to be observed was not observed because it was overlapped the broadband belonging to the π-π * transition.

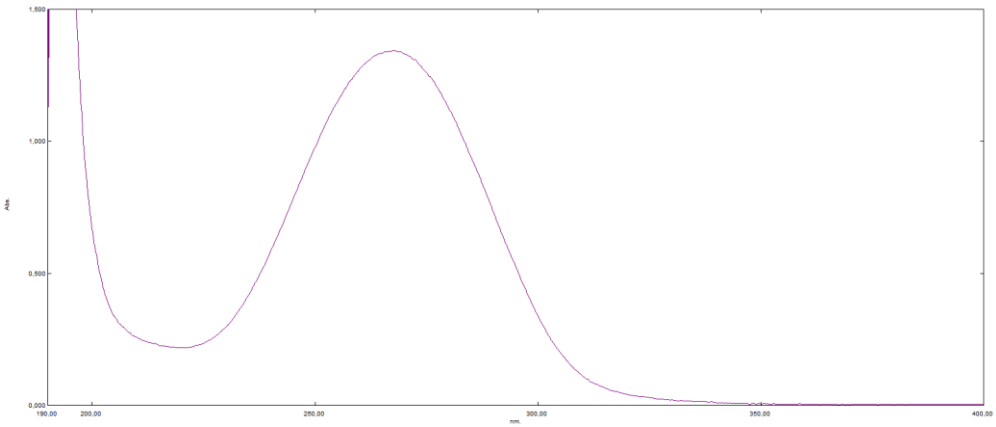


Figure 2. The experimental UV–Vis spectrum of molecule **3**.

Theoretically calculated UV spectrum with DFT B3LYP/6-311+G(d,p) is as in Figure 3. Since it was not in harmony with the experimental UV spectrum, the spectrum was taken again in buffer solutions prepared in notr (pH 7), acidic (pH 1), and basic (pH 13) buffer solutions experimentally. It was observed that the spectrum taken at pH 7 showed two peaks similar to the theoretically acquired spectrum (Figure 4)

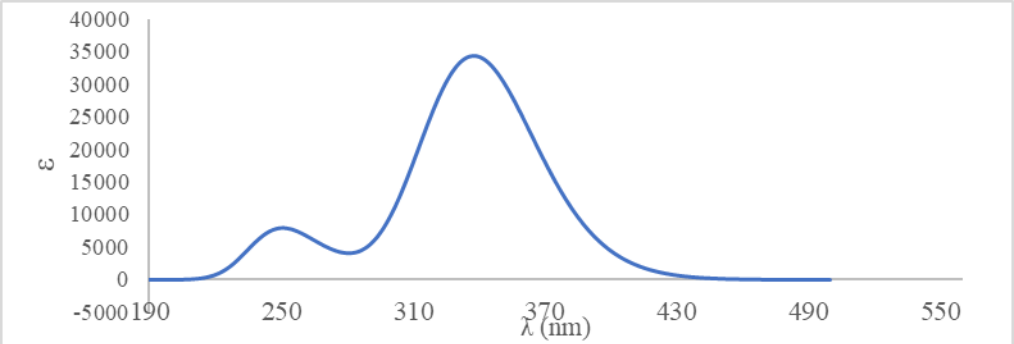


Figure 3. The theoretical UV–Vis spectrum of molecule 3.

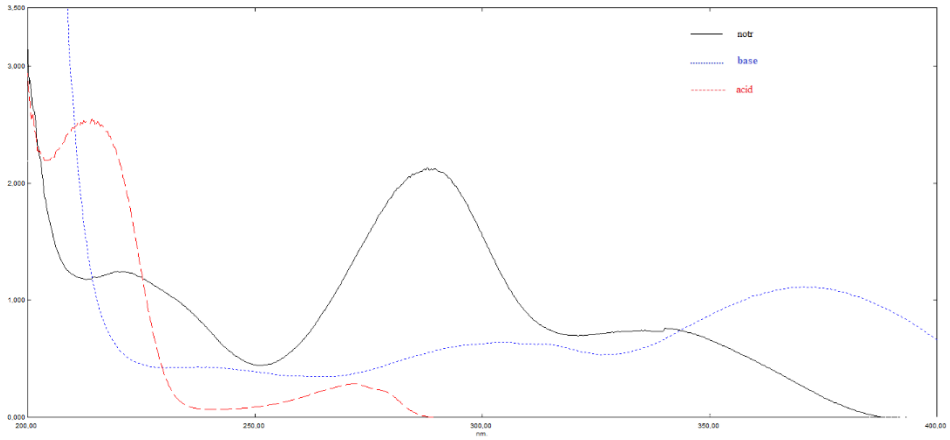


Figure 4. The experimental UV spectrum of molecule **3** in notr (pH 7), acidic (pH 1) and basic (pH 13) buffer solutions.

4.1.2. Vibrational spectroscopy (IR)

FT-IR spectra of molecule 3 was obtained using the KBr disk (Figure 5). The aromatic structure shows the presence of C–H stretching vibrations in the region 3144-3069 cm^{-1}, which is the characteristic region for ready identification of C–H stretching vibrations. The phenolic group O-H shows a stretching band in the 3280 cm^{-1} range. The C=C stretching peaks in the aromatic rings are observed between the 1581-1444 cm^{-1} range. The C-O stretching band of the phenol is found in the range of 1247 cm^{-1}. The C=N stretching frequency is found at 1621 cm^{-1}.The N-H peak that should be observed in the imidazole ring could not be observed because it overlapped the phenolic group O-H peak.

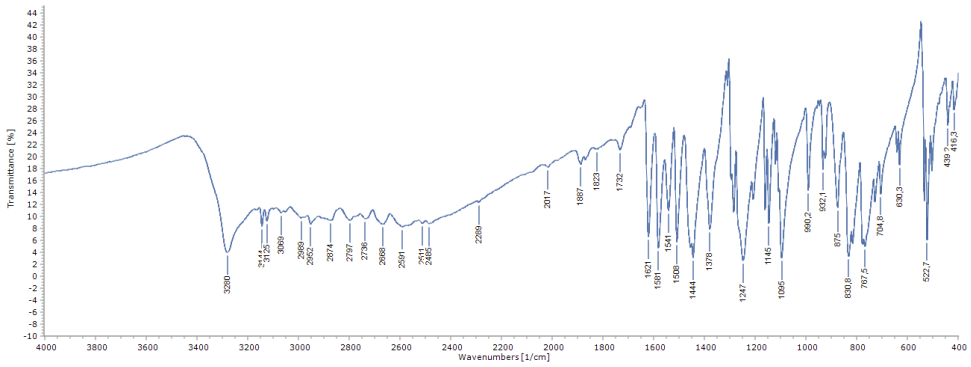


Figure 5. The experimental IR spectrum of molecule **3**

Theoretical infrared calculations of compound 3 were performed on the DFT B3LYP/6-311+G(d,p) base set. The Infrared Bands are visualized with the Gauss-View program and summarized in Table 1. Although the results obtained and the experimental data are generally in agreement, the experimental data. When the data were compared, it was determined that the theoretical values were insufficient. The main reason for this is that while there are intermolecular interactions in the experimental data, the theoretical calculations are carried out on a single molecule and the theoretical calculations are taken in the gas phase while the experimental data are taken in the solid state (Figure 6).

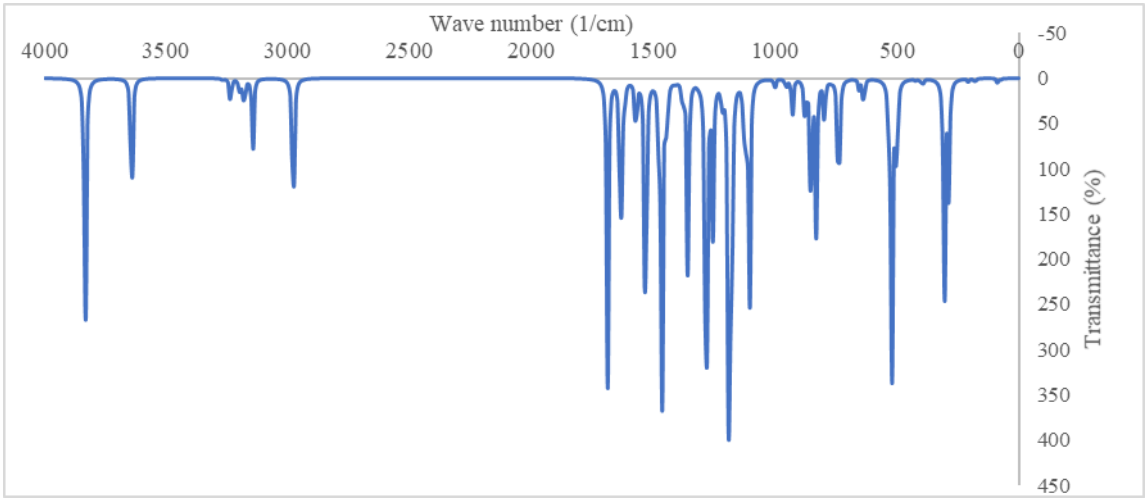


Figure 6: The theoretical IR spectrum of molecule **3**.

Table 1. The experimental and theoretical characteristic IR frequencies (cm^{-1}) of molecule **3**.

	Experimental $\nu(cm^{-1})$	Theoretical $\nu(cm^{-1})$
υ O-H (aromatic)	3280	3834.17
υ N-H (iminee)	Not observed (It was not observed because it remained below the O-H peak)	3643.24
υ C-H (aromatic imidazole ring)	3165 3144	3268.74 3237.34
υ C-H (aromatic benzene ring)	3125 3069 3051	3201.69 3187.41 3180.00 3145.50
υ N-H (imine)	2989	2979.52
υ C=N (imine)	1621	1688.37
υ C=C (benzene ring)	1581 1541 1508	1635.15 1620.62 1523.78
υ C=C (imidazole ring)	1455 1444	1572.50 1476.61 1465.20
υ C-O (aromatic)	1247	1283.62

The correlation of theoretical and experimental IR spectra was found to be 0.99 (Figure 7).

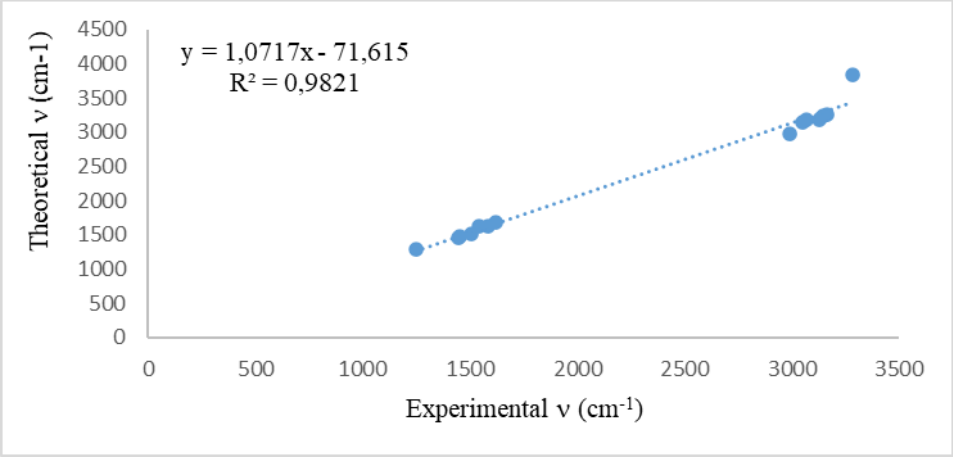
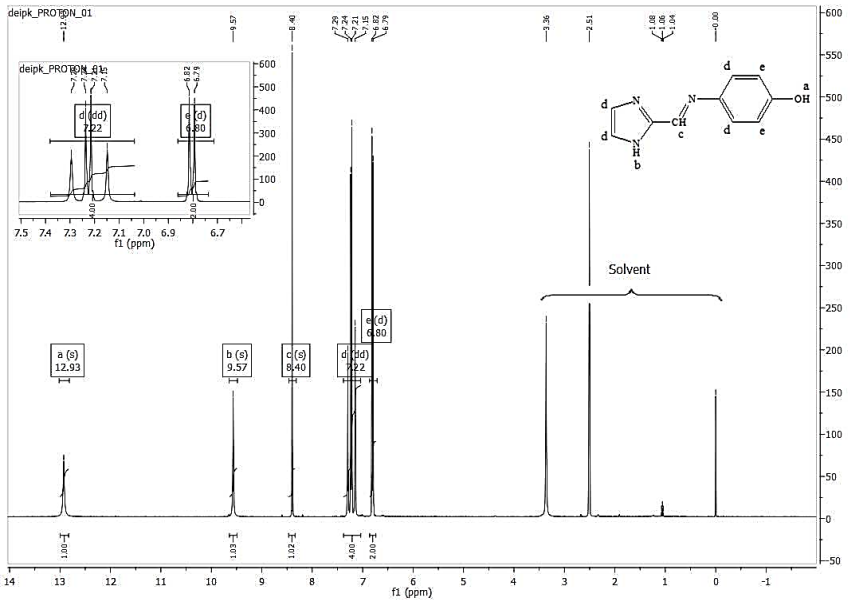


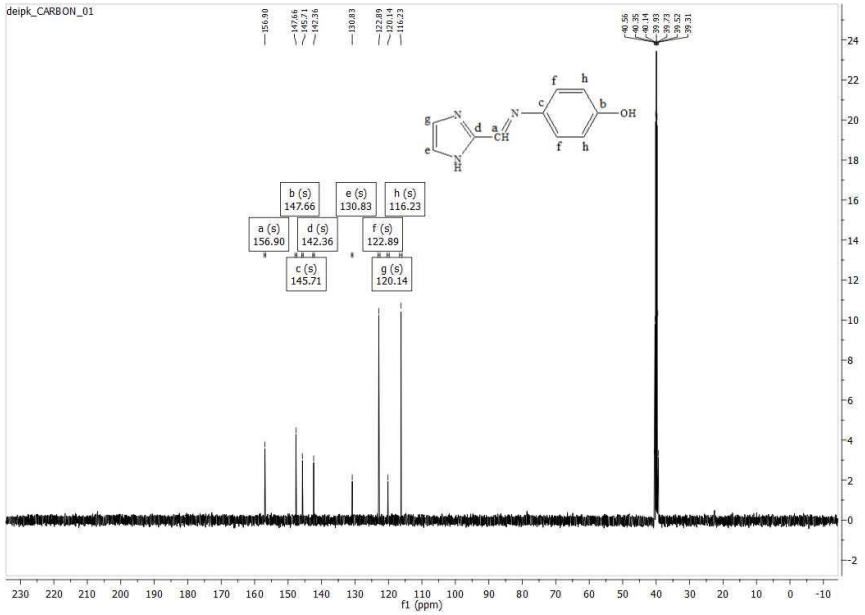
Figure 7. The correlation graph of the experimental and theoretical vibrational IR frequencies of molecule 3.

4.1.3. ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy (NMR)

The experimental ^{1}H and ^{13}C NMR spectral data of the molecule are shown in Figure 8. The ^{1}H NMR spectrum of the Schiff base ligand was recorded in DMSO-d_6. In the ^{1}H NMR spectra of Schiff base ligand, the peaks appeared at 7.22 and 6.80 ppm were assigned to the proton of the phenolic group, singlet peaks appeared at 7.27 and 7.13 were assigned to the imidazole, and singlet peaks appeared at 8.40 ppm were assigned to protons of imine group. The ^{13}C NMR spectrum of the Schiff base ligand was recorded in DMSO-d_6. In the ^{13}C-NMR spectra of the molecule, the signal that appeared at 156.90 ppm was assigned to imine carbon atoms (C=N). A signal at 147.66, 145.71, 122.89, and 116.23 ppm were assigned for phenolic carbon. The carbons of the imidazole were observed at 142.36, 130.83, and 120.14 ppm.



(a)

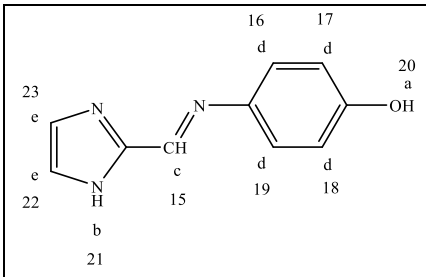


(b)

Figure 8. ^{1}H (a) and ^{13}C (b) NMR spectra of molecule **3** in DMSO- d_6 were obtained experimentally.

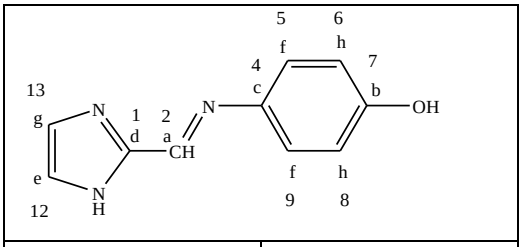
Experimental NMR analysis was taken in 400 MHz NMR device in DMSO-d6 solvent environment, and theoretical NMR analysis was taken in B3LYP / GIAO model set and the values were summarized in Table 2 and Table 3. When the experimental and theoretical NMR values are compared, the equation at ^{1}H-NMR is y = 1,1276x-1,0639; R^2 = 0,5954 while in ^{13}C-NMR the equation is y = 0,6923+56,321; R^2 = 0.4326. When R^2 values are examined, bad harmony is observed in theoretical and experimental values; It can be said that this value in ^{1}H-NMR is lower since acidic protons are more mobile than other protons.

Table 2. ^{1}H chemical shifts δ [ppm] determined as experimental and theoretical for molecule **3**.



Theoretical		Experimental	
Atom	Chemical Shift	Atom	Chemical Shift
20H	3.99	a (1H, s)	12.93
21H	8.43	b (1H, s)	8.40
15H	8.98	c (1H, s)	9.57
16H 19H 22H 23H	8.06 7.81 7.26 7.75	d (4H, dd)	7.22
17H 18H	7.32 6.71	e (2H, d)	6.80

Table 3. ^{13}C NMR chemical shifts δ [ppm] determined as experimental and theoretical for molecule **3**.



Experimental		Theoretical	
Atom	Chemical Shift	Atom	Chemical Shift
C2	156.90	a (s)	150.47
C7	147.66	b (s)	175.16
C4	145.71	c (s)	1 58.71
C1	142.36	d (s)	162.88
C12	130.83	e (s)	131.31
C5 C9	122.89	f (s)	153.59 127.60
C13	120.14	g (s)	150.91
C6 C8	116.23	h (s)	131.99 128.12

4.2. Theoretical Results

4.3. Energy, Dipole and Mulliken Atomic Charge Values

Dipole moment, polarization, and acid-base behavior of a molecule are affected by atomic charges. Therefore Mulliken atomic charge calculations play an important role in chemical calculations. The Mulliken atomic charges were listed in Table 5. Accordingly, the most negative atom observed as oxygen bound to the benzene ring. Although, usually, heteroatoms and the carbon atoms attached to them are determined negatively, the most positive atom is in the benzene ring observed as the numbered nine carbon atom.
Dipole moment is an important parameter in chemistry and shows charge transfer across the molecule. Dipole moment for **3** was calculated as 6.031 D (Table 4). If the net dipole moment is greater than zero, the bond and molecule are considered polar. They tend to form chemical bonds with atoms that have similar electronegativity values.

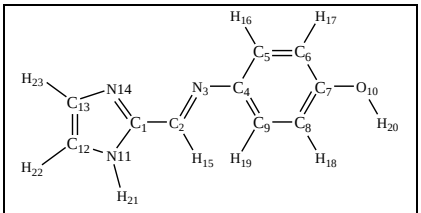
Zero-point energy is the lowest energy a physical system can have in quantum mechanics. Zero-point energy of the molecule determined 110,527 kcal/mol and Sum of electronic and thermal Free Energies determines -392800,817 kcal/mol.

Table 4. The zero-point energy, thermal free energies, and dipole moment of molecule **3**.

Zero-point vibrational energy (Kcal/Mol)	110,527
Sum of electronic and thermal Free Energies* (Kcal/Mol)	-392800,817
Dipole moment (Debye)	6,031

*1 Hatree=627.509 kcal/Mol

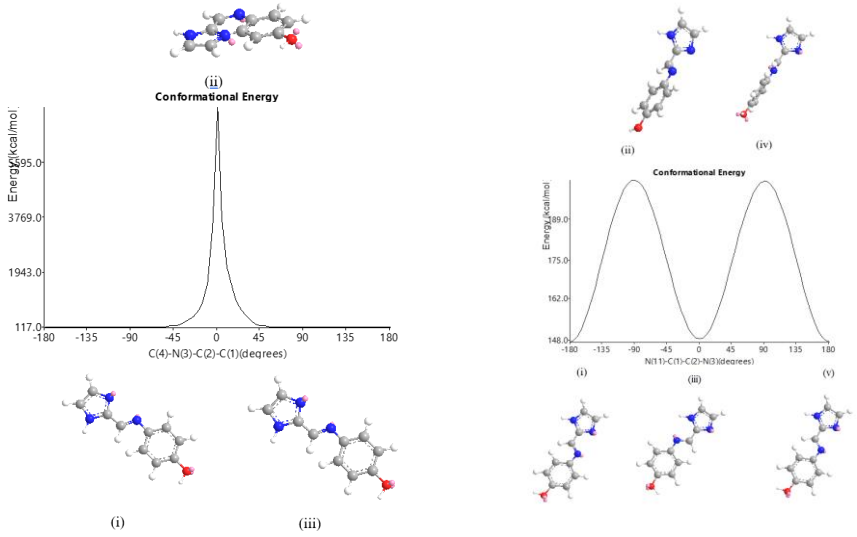
Table 5. The Mulliken atomic charges of molecule **3**.



Atom	Mulliken atomic charges
1C	-0.136
2C	-0.253
3N	0.096
4C	-0.333
5C	-0.216
6C	-0.022
7C	-0.491
8C	-0.170
9C	0.359
10O	-0.230
11N	-0.113
12C	-0.230
13C	0.240
14N	-0.130
15H	0.068
16H	0.209
17H	0.196
18H	0.150
19H	0.104
20H	0.265
21H	0.284
22H	0.165
23H	0.186

4.3.1. pK$_a$ Calculation

Formation enthalpies of the cis and trans forms of the molecule were calculated (Figure 9). Since the formation enthalpy of cis form is very high, we decided to make the pKa calculations on trans form. We calculated the acidity constant in trans form with the lowest energy dihedral angle.



(a) (b)

Figure 9. Calculated lowest energy dihedral angle graphics of the studied molecule's cis (a) and trans (b) forms.

Theoretical acidity constants have been made by considering the protonation and deprotonation center (Figure 10) of the molecule were calculated in the Gaussian09 program at the level of DFT method B3LYP/6-311++G(d,p) according to equation 3 (Table 6) [33].

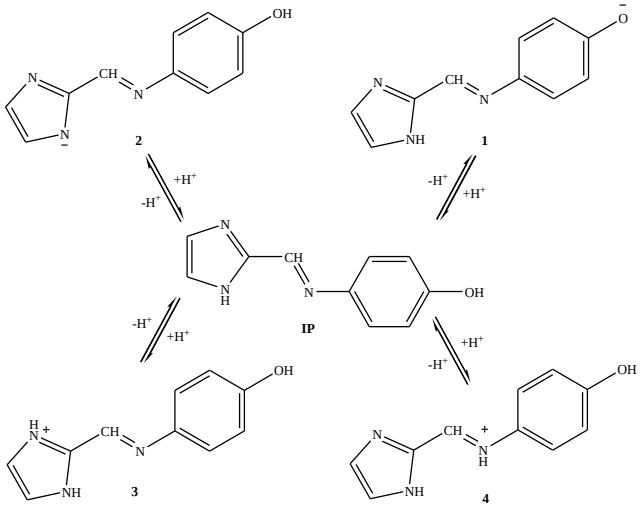


Figure 10. The protonated and deprotonated forms of the studied molecule are shown in the Scheme.

Table 6. The calculated pK_a values of the molecule **3**

Molecule	BH^+s	Bs	BH^+g	Bg	ΔGs	ΔGg	δΔG(BH^+)	pKa calc.
1	-392671.493	-392367.041	-392656.924	-392310.175	-68.632	-182.030	-250.662	2.2643
2	-392675.164	-390298.145	-392665.648	-390242.205	-2141.199	-2258.723	-4399.922	3.5087
3	-392963.744	-392671.493	-392916.720	-392656.924	-56.431	-95.076	-151.506	2.0457
4	-392960.689	-392671.493	-392913.094	-392656.924	-53.376	-91.450	-144.825	2.0261

Deviation= Experimental pK_a- Calculated pK_a

Values of pKa were predicted using MarvinSketchTM 5.3.7 (ChemAxon Ltd., Budapest, Hungary; www.chemaxon.com) and MOPAC2016. The fact that the MOPAC2016 calculations are compatible with the 1 data from different conformations made for MarvinSketch (ChemAxon), shows that these methods are in harmony. The theoretically were calculated pK_a values of the molecule studied are given in Table 7.

Table7. The calculated pK_a values of the molecule **3**

Molecule 3	Method	pKa
A	MOPAC2016	8.244
A	MarvinSketch	8.019
B		11.746
C		5.588
D		0.403
A		2.2643
	DFT	
B		3.508
C		2.045
D		2.026

4.3.2. HOMO-LUMO

The Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) play a key role in the determination of molecular properties [34]. HOMO-LUMO energy values and energy maps represent the chemical activity and kinetic stability of the molecule. HOMO and LUMO surfaces and energies of the molecule was calculated in the gas phase and B3LYP/6-311+G(d,p) level in different solvents and the results obtained are given in Figure 11. When the HOMO values of the obtained compound were examined, it was determined that the electron density was distributed over the whole compound.

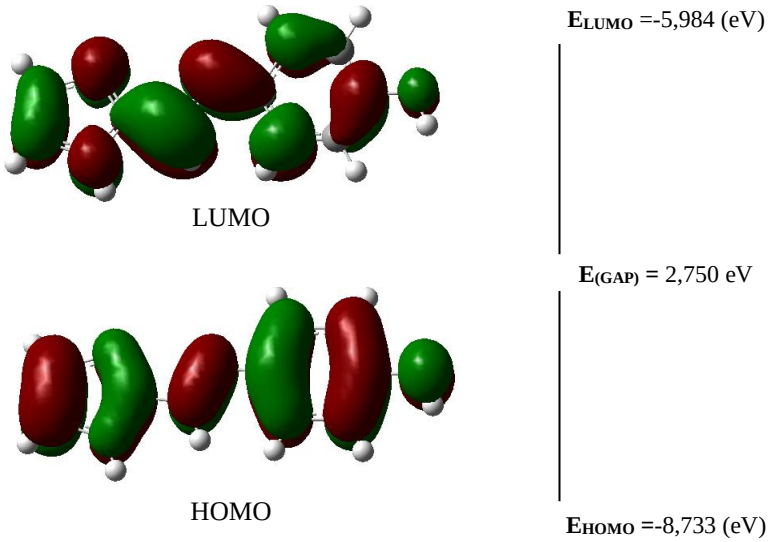


Figure 11. HOMO and LUMO 3D plots of molecule 3 were obtained with the B3LYP/6-311 + g(d, p) method.

Chemical hardness and softness are important parameters for the stability and reactivity of the molecule. Hard molecules have large energy values soft molecules have small energy values. Soft molecules are more reactive than hard molecules because they can easily present their electrons to a receptor. Other molecular parameters can be associated with these values. Accordingly, the low HOMO-LUMO values of the obtained compound indicate that the reaction activity will be easier and it can easily bind to metal atoms or a receptor.

4.3.3. Molecular electrostatic potential (MEP) surface analysis

The Molecular Electrostatic Potential (MEP) is an optical method that provides information about the net electrostatic effect created by the total charge distribution in the molecule, as well as the electronegativity of a compound, its charge, dipole moment, and its ratio to the chemical reaction while allowing us to understand the molecular polarity [35]. The different colors of the resulting compound dimensionally are shown in the MEP map. In colors, the blue color indicates positive regions of the molecule, green color indicates mild regions and red color indicates negative regions. The MEP surface of the molecule was plotted using the 6-311 + G(d, p) based DFT / B3LYP level adjusted to estimate the reactive sites of the electrophilic and nucleophilic attack on the molecule investigated (Figure 12). According to this, the regions of the compound, especially the regions where oxygen and nitrogen atoms are rich in electrons, are the places where hydrogen atoms are seen as positive.

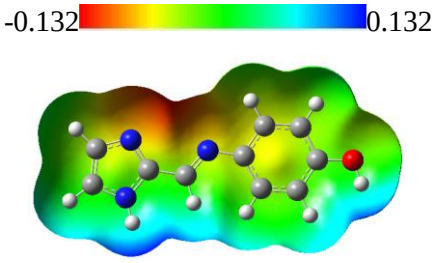


Figure 12. MEP 3D plot of molecule 3 obtained with B3LYP/6-311 + g(d, p) method.

4.3.4. Solvent Accessibility Surface (SAS)

The solvent accessibility surface of the compound is given in Figure 13. SAS, showing regions of interaction with the solvent, is very useful for describing specific solute-solvent interactions. The red regions indicate the regions where polar or polar protic solvents will interact with the oxygen atom in the compounds. The blue regions indicate the regions where polar or polar protic solvents will interact with the nitrogen atom in the compounds. Green regions indicate the regions where polar or polar protic solvents will interact with the -Cl atom in the compound. Gray regions indicate the regions where apolar solvents will interact with benzene rings and other saturated hydrocarbons in the compound. Compounds appear to interact with polar or polar protic solvents, polar atoms (N, O, and S), and apolar solvents with low polarity atoms (C).

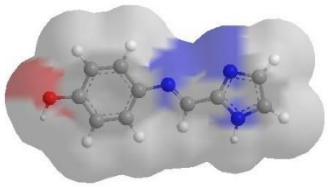


Figure 13. MEP 3D plot of molecule 3

4.3.5. Dielectric Constant

The dielectric coefficient (dielectric constant) can be defined as the ratio of the permittivity of the medium to the permittivity of the free space. Permeability is the quality that describes the effect of a material on an electric field. The higher the permeability, the more the material tends to reduce the area created in that area. Materials with a high dielectric constant have a strong ability to become polarized. If the polarization developed by applying an electric field is high for a dielectric material, the dielectric constant will also be high. The higher the resistance to electric current flow, the higher the dielectric constant.

For this molecule, the isoelectric point was found to be 6.92 as a result of the calculations we made in the Marven program.

5. CONCLUSION

In this study, the synthesis of 4-(((1H-imidazole-2-yl)methylene)amino)phenol (IP) compound was performed for the first time in the literature. The structure of the obtained compound was illuminated by ^{1}H-NMR, ^{13}C-NMR, IR, UV-Vis, and elemental analysis techniques. In the second stage of the study, the theoretical calculations of the compound were made with the Gaussian 09 program. Experimental and theoretical IR and UV-Vis values were generally in harmony.

We aimed to contribute with theoretical studies, thinking that the synthesized structure could be used as a drug in future studies. One of the most important factors in the attachment of a molecule to a biological target is its conformation. For this reason, all theoretical studies have been based on the lowest energy conformation. The acid-base dissociation constant (pKa) of a drug is an important physicochemical parameter that affects many biopharmaceutical properties. The pKa distributions of drugs are affected by two main factors. The first relates to the nature and frequency of formation of functional groups commonly observed in pharmaceuticals and the typical range of pKa values they emit. The other factor has to do with the biological targets these compounds are designed to hit. Determination of the pKa value in terms of examining the active drug property of the synthesized structure in this study was determined theoretically because it is important for future studies. Since its conductivity is 6.92, it was thought that the studied material could be used as an insulator.

ACKNOWLEDGMENTS

The theoretical calculations in this study were carried out on a computer taken from Anadolu University 1309F20 BAP project.

CONFLICT OF INTEREST

The authors stated that there are no conflicts of interest regarding the publication of this article.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

ALMOST CONTACT STRUCTURES ON SOME LIE ALGEBRAS

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ABSTRACT

In this manuscript, we show that there are no almost contact structures with parallel characteristic vector field on certain 7 dimensional Lie algebras over the real field.

Keywords: 7-dimensional nilpotent Lie algebra, Almost contact metric structure, Parallel vector field

1. INTRODUCTION

Determining possible left invariant almost contact structures on Lie groups or on Lie algebras corresponding to these gropus is a recent research area. In 3-dimensions, almost contact metric structures which are homogeneous were studied by [1]. In [2], it was shown that the real Heisenberg group is the only odd dimensional nilpotent Lie group with a left-invariant Sasakian structure. Also, Sasakian Lie algebras were classified in 5 dimensions. K-contact structures on 5-dimensional Lie groups were given in [3]. In [4], existences of cosymplectic, nearly cosymplectic, α −Sasakian, β −Kenmotsu, almost cosymplectic and semi-cosymplectic structures were studied on 5 dimensions. In [5], quasi-Sasakian structures on nilpotent Lie algebras were investigated in five dimensions. After the classification of 7-dimensional nilpotent Lie algebras by [6], there have been studies on almost contact metric structures on 7-dimensional nilpotent Lie algebras, see [7, 8, 9].

In this work we study almost contact metric structures having parallel characteristic vector field on indecomposable 7-dimensional nilpotent Lie algebras over the real field.

2. PRELIMINARIES

An almost contact structure (ϕ, ξ, η) on an odd dimensional manifold M consists of a vector field ξ, a 1-form η on M and an endomorphism ϕ such that

$$\phi^2 = -I + \eta \otimes \xi, \qquad \eta(\xi) = 1.$$

In addition, if M also has a Riemannian metric g satisfying

$$g(\phi(X), \phi(Y)) = g(X, Y) - \eta(X)\eta(Y)$$

for all vector fields X, Y, then M is said to be an almost contact metric manifold.

Almost contact metric manifolds were classified into 2^{12} classes due to symmetries of the covariant derivative of the fundamental 2-form, see [10] and [11]. The class of cosymplectic manifolds is the trivial class with the defining relation $\nabla\Phi = 0$ [12].

There are 12 basic classes C_i, i=1,…,12 and all classes are direct sums of these basic classes [10]. It can be seen from the defining relations of these classes that for an almost contact structure in C_1, C_2, C_3, C_4 and C_{11}, the characteristic vector field ξ of the almost contact metric structure is parallel. In this study

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we show that none of the 7-dimensional indecomposable nilpotent Lie algebras over the real field $\mathbb{R}$ has a parallel vector field. Thus there are no almost contact metric structures of classes C_1, C_2, C_3, C_4 and C_{11}.

A left invariant almost contact metric structure (ϕ, ξ, η, g) on a connected Lie group L induces an almost contact metric structure (ϕ, ξ, η, g) on the corresponding Lie algebra ℓ of L, see [13]. We denote the structure on ℓ also by (ϕ, ξ, η, g).

3. ALMOST CONTACT STRUCTURES WITH PARALLEL VECTOR FIELD

Assume that $(\boldsymbol{\phi}, \boldsymbol{\xi}, \boldsymbol{\eta}, \boldsymbol{g})$ is an almost contact metric structure on a 7-dimensional indecomposable nilpotent Lie algebra over $\mathbb{R}$. For the list of these algebras, refer to [6].

Theorem There is no almost contact metric structure with parallel characteristic vector field on an indecomposable nilpotent Lie algebra over $\mathbb{R}$ in dimension 7.

Proof We give the proof for Lie algebras with upper central series dimensions 37. Calculations for other series with upper central series dimensions 357, 27, 257, 247, 2457, 2357, 23457, 17, 157, 147, 1457, 137, 1357, 13457, 12457, 12357, 123457 are similar. We show that none of the algebras in [6] has a parallel vector field.

The Lie algebra 37A**:**

Consider the Lie algebra $\boldsymbol{37A}$ in the list of [6] with upper central series dimension 37. Assume that $(\boldsymbol{\phi}, \boldsymbol{\xi}, \boldsymbol{\eta}, \boldsymbol{g})$ is an almost contact metric structure on $\boldsymbol{37A}$. Choose the $\boldsymbol{g}$-orthonormal basis $\{\boldsymbol{b_1}, \dots, \boldsymbol{b_7}\}$ of this Lie algebra. The non-zero brackets are

$$[\boldsymbol{b_1}, \boldsymbol{b_2}] = \boldsymbol{b_5}, [\boldsymbol{b_2}, \boldsymbol{b_3}] = \boldsymbol{b_6}, [\boldsymbol{b_2}, \boldsymbol{b_4}] = \boldsymbol{b_7}.$$

We write the nonzero covariant derivatives by the Kozsul's formula.

$$\begin{aligned}
&\boldsymbol{\nabla_{b_1} b_2 = \frac{1}{2} b_5}, \quad \boldsymbol{\nabla_{b_1} b_5 = -\frac{1}{2} b_2}, \quad \boldsymbol{\nabla_{b_2} b_1 = -\frac{1}{2} b_5}, \quad \boldsymbol{\nabla_{b_2} b_3 = \frac{1}{2} b_6},\\
&\boldsymbol{\nabla_{b_2} b_4 = \frac{1}{2} b_7}, \quad \boldsymbol{\nabla_{b_2} b_5 = \frac{1}{2} b_1}, \quad \boldsymbol{\nabla_{b_2} b_6 = -\frac{1}{2} b_3}, \quad \boldsymbol{\nabla_{b_2} b_7 = -\frac{1}{2} b_4},\\
&\boldsymbol{\nabla_{b_3} b_2 = -\frac{1}{2} b_6}, \quad \boldsymbol{\nabla_{b_3} b_6 = \frac{1}{2} b_2}, \quad \boldsymbol{\nabla_{b_4} b_2 = -\frac{1}{2} b_7}, \quad \boldsymbol{\nabla_{b_4} b_7 = \frac{1}{2} b_2},\\
&\boldsymbol{\nabla_{b_5} b_1 = -\frac{1}{2} b_2}, \quad \boldsymbol{\nabla_{b_5} b_2 = \frac{1}{2} b_1}, \quad \boldsymbol{\nabla_{b_6} b_2 = -\frac{1}{2} b_3}, \quad \boldsymbol{\nabla_{b_6} b_3 = \frac{1}{2} b_2},\\
&\boldsymbol{\nabla_{b_7} b_2 = -\frac{1}{2} b_4}, \quad \boldsymbol{\nabla_{b_7} b_4 = \frac{1}{2} b_2}.
\end{aligned}$$

Let $\boldsymbol{\xi = \sum a_i b_i}$ be a parallel vector field on $\boldsymbol{37A}$. Then for all basis elements, we have $\boldsymbol{\nabla_{b_i} \xi = 0}$.

$$\boldsymbol{0 = \nabla_{b_1} \xi = \nabla_{b_1}(a_1 b_1 + \cdots + a_7 b_7) = \frac{a_2}{2} b_5 - \frac{a_5}{2} b_2}$$

implies $\boldsymbol{a_2 = a_5 = 0}$ from linear independence of vectors $\boldsymbol{b_5}$ and $\boldsymbol{b_2}$.

$$\boldsymbol{0 = \nabla_{b_2} \xi = \nabla_{b_2}(a_1 b_1 + \cdots + a_7 b_7) = -\frac{a_1}{2} b_5 + \frac{a_3}{2} b_6 + \frac{a_4}{2} b_7 + \frac{a_5}{2} b_1 - \frac{a_6}{2} b_3 - \frac{a_7}{2} b_4}$$

gives that remaining constants $\boldsymbol{a_i}$ are also zero.

The Lie algebra 37B:

Non-zero brackets of $\boldsymbol{g}$-orthonormal basis elements $\{\boldsymbol{b_1}, \dots, \boldsymbol{b_7}\}$ are

$$[\boldsymbol{b_1}, \boldsymbol{b_2}] = \boldsymbol{b_5}, [\boldsymbol{b_2}, \boldsymbol{b_3}] = \boldsymbol{b_6}, [\boldsymbol{b_3}, \boldsymbol{b_4}] = \boldsymbol{b_7}$$

and the nonzero covariant derivatives are:

$$\begin{aligned}
&\nabla_{b_1} b_2 = \frac{1}{2} b_5, \quad \nabla_{b_1} b_5 = -\frac{1}{2} b_2, \quad \nabla_{b_2} b_1 = -\frac{1}{2} b_5, \quad \nabla_{b_2} b_3 = \frac{1}{2} b_6,\\
&\nabla_{b_2} b_5 = \frac{1}{2} b_1, \quad \nabla_{b_2} b_6 = -\frac{1}{2} b_3, \quad \nabla_{b_3} b_2 = -\frac{1}{2} b_6, \quad \nabla_{b_3} b_4 = \frac{1}{2} b_7,\\
&\nabla_{b_3} b_6 = \frac{1}{2} b_2, \quad \nabla_{b_3} b_7 = -\frac{1}{2} b_4, \quad \nabla_{b_4} b_3 = -\frac{1}{2} b_7, \quad \nabla_{b_4} b_7 = \frac{1}{2} b_3,\\
&\nabla_{b_5} b_1 = -\frac{1}{2} b_2, \quad \nabla_{b_5} b_2 = \frac{1}{2} b_1, \quad \nabla_{b_6} b_2 = -\frac{1}{2} b_3, \quad \nabla_{b_6} b_3 = \frac{1}{2} b_2,\\
&\nabla_{b_7} b_3 = -\frac{1}{2} b_4, \quad \nabla_{b_7} b_4 = \frac{1}{2} b_3.
\end{aligned}$$

Let $\boldsymbol{\xi} = \sum \boldsymbol{a_i} \boldsymbol{b_i}$ be a parallel vector field on $\boldsymbol{37B}$. Then from equations $\nabla_{b_i} \boldsymbol{\xi} = \boldsymbol{0}$, we obtain the followings.

$$\boldsymbol{0} = \nabla_{b_1} \boldsymbol{\xi} = \frac{\boldsymbol{a_2}}{\boldsymbol{2}} \boldsymbol{b_5} - \frac{\boldsymbol{a_5}}{\boldsymbol{2}} \boldsymbol{b_2}$$

implies $\boldsymbol{a_2} = \boldsymbol{a_5} = \boldsymbol{0}$.

$$\boldsymbol{0} = \nabla_{b_2} \boldsymbol{\xi} = -\frac{\boldsymbol{a_1}}{\boldsymbol{2}} \boldsymbol{b_5} + \frac{\boldsymbol{a_3}}{\boldsymbol{2}} \boldsymbol{b_6} + \frac{\boldsymbol{a_5}}{\boldsymbol{2}} \boldsymbol{b_1} - \frac{\boldsymbol{a_6}}{\boldsymbol{2}} \boldsymbol{b_3}$$

gives that $\boldsymbol{a_1} = \boldsymbol{a_3} = \boldsymbol{a_6} = \boldsymbol{0}$.

From the equation

$$\boldsymbol{0} = \nabla_{b_3} \boldsymbol{\xi} = \frac{\boldsymbol{a_4}}{\boldsymbol{2}} \boldsymbol{b_7} - \frac{\boldsymbol{a_7}}{\boldsymbol{2}} \boldsymbol{b_4},$$

we get $\boldsymbol{a_4} = \boldsymbol{a_7} = \boldsymbol{0}$. Thus $\boldsymbol{\xi} = \boldsymbol{0}$.

The algebra 37C:

The non-zero brackets are

$$[\boldsymbol{b_1}, \boldsymbol{b_2}] = \boldsymbol{b_5}, [\boldsymbol{b_2}, \boldsymbol{b_3}] = \boldsymbol{b_6}, [\boldsymbol{b_2}, \boldsymbol{b_4}] = \boldsymbol{b_7}, [\boldsymbol{b_3}, \boldsymbol{b_4}] = \boldsymbol{b_5}$$

and the nonzero covariant derivatives are:

$$\begin{aligned}
&\nabla_{b_1} b_2 = \frac{1}{2} b_5, \quad \nabla_{b_1} b_5 = -\frac{1}{2} b_2, \quad \nabla_{b_2} b_1 = -\frac{1}{2} b_5, \quad \nabla_{b_2} b_3 = \frac{1}{2} b_6,\\
&\nabla_{b_2} b_4 = \frac{1}{2} b_7, \quad \nabla_{b_2} b_5 = \frac{1}{2} b_1, \quad \nabla_{b_2} b_6 = -\frac{1}{2} b_3, \quad \nabla_{b_2} b_7 = -\frac{1}{2} b_4,\\
&\nabla_{b_3} b_2 = -\frac{1}{2} b_6, \quad \nabla_{b_3} b_4 = \frac{1}{2} b_5, \quad \nabla_{b_3} b_5 = -\frac{1}{2} b_4, \quad \nabla_{b_3} b_6 = \frac{1}{2} b_2,\\
&\nabla_{b_4} b_2 = -\frac{1}{2} b_7, \quad \nabla_{b_4} b_3 = -\frac{1}{2} b_5, \quad \nabla_{b_4} b_5 = \frac{1}{2} b_3, \quad \nabla_{b_4} b_7 = \frac{1}{2} b_2,
\end{aligned}$$

$$\nabla_{b_5} b_1 = -\frac{1}{2} b_2, \quad \nabla_{b_5} b_2 = \frac{1}{2} b_1, \quad \nabla_{b_5} b_3 = -\frac{1}{2} b_4, \quad \nabla_{b_5} b_4 = \frac{1}{2} b_3,$$

$$\nabla_{b_6} b_2 = -\frac{1}{2} b_3, \quad \nabla_{b_6} b_3 = \frac{1}{2} b_2, \quad \nabla_{b_7} b_2 = -\frac{1}{2} b_4, \quad \nabla_{b_7} b_4 = \frac{1}{2} b_2.$$

Let $\xi = \sum a_i b_i$ be a parallel vector field on $\mathbf{37C}$. Checking the condition $\nabla_{b_i} \xi = 0$ for all basis elements, we get that

$$0 = \nabla_{b_1} \xi = \frac{a_2}{2} b_5 - \frac{a_5}{2} b_2$$

which implies $a_2 = a_5 = 0$ and

$$0 = \nabla_{b_2} \xi = -\frac{a_1}{2} b_5 + \frac{a_3}{2} b_6 + \frac{a_4}{2} b_7 + \frac{a_5}{2} b_1 - \frac{a_6}{2} b_3 - \frac{a_7}{2} b_4$$

gives that remaining constants are also zero.

The algebra $\mathbf{37D}$:

The non-zero brackets are

$$[b_1, b_2] = b_5, [b_1, b_3] = b_6, [b_2, b_4] = b_7, [b_3, b_4] = b_5$$

and the nonzero covariant derivatives are:

$$\nabla_{b_1} b_2 = \frac{1}{2} b_5, \quad \nabla_{b_1} b_3 = \frac{1}{2} b_6, \quad \nabla_{b_1} b_5 = -\frac{1}{2} b_2, \quad \nabla_{b_1} b_6 = -\frac{1}{2} b_3,$$
$$\nabla_{b_2} b_1 = -\frac{1}{2} b_5, \quad \nabla_{b_2} b_4 = \frac{1}{2} b_7, \quad \nabla_{b_2} b_5 = \frac{1}{2} b_1, \quad \nabla_{b_2} b_7 = -\frac{1}{2} b_4,$$

$$\nabla_{b_3} b_1 = -\frac{1}{2} b_6, \quad \nabla_{b_3} b_4 = \frac{1}{2} b_5, \quad \nabla_{b_3} b_5 = -\frac{1}{2} b_4, \quad \nabla_{b_3} b_6 = \frac{1}{2} b_1,$$
$$\nabla_{b_4} b_2 = -\frac{1}{2} b_7, \quad \nabla_{b_4} b_3 = -\frac{1}{2} b_5, \quad \nabla_{b_4} b_5 = \frac{1}{2} b_3, \quad \nabla_{b_4} b_7 = \frac{1}{2} b_2,$$
$$\nabla_{b_5} b_1 = -\frac{1}{2} b_2, \quad \nabla_{b_5} b_2 = \frac{1}{2} b_1, \quad \nabla_{b_5} b_3 = -\frac{1}{2} b_4, \quad \nabla_{b_5} b_4 = \frac{1}{2} b_3,$$
$$\nabla_{b_6} b_1 = -\frac{1}{2} b_3, \quad \nabla_{b_6} b_3 = \frac{1}{2} b_1, \quad \nabla_{b_7} b_2 = -\frac{1}{2} b_4, \quad \nabla_{b_7} b_4 = \frac{1}{2} b_2.$$

Let $\xi = \sum a_i b_i$ be a parallel vector field on $\mathbf{37D}$. Then since $\nabla_{b_i} \xi = 0$ for all basis elements, we obtain

$$0 = \nabla_{b_1} \xi = \frac{a_2}{2} b_5 + \frac{a_3}{2} b_6 - \frac{a_5}{2} b_2 - \frac{a_6}{2} b_3$$

implying $a_2 = a_3 = a_5 = a_6 = 0$ and

$$0 = \nabla_{b_2} \xi = -\frac{a_1}{2} b_5 + \frac{a_4}{2} b_7 - \frac{a_7}{2} b_4$$

gives that remaining constants are also zero.

The algebra $\mathbf{37B_1}$:

The non-zero brackets are
$[b_1, b_2] = b_5, [b_1, b_3] = b_6, [b_1, b_4] = b_7, [b_2, b_4] = b_6, [b_3, b_4] = -b_5.$

Some of the nonzero covariant derivatives are:

$$\nabla_{b_1} b_2 = \frac{1}{2} b_5, \quad \nabla_{b_1} b_3 = \frac{1}{2} b_6, \quad \nabla_{b_1} b_4 = \frac{1}{2} b_7, \quad \nabla_{b_1} b_5 = -\frac{1}{2} b_2,$$
$$\nabla_{b_1} b_6 = -\frac{1}{2} b_3, \quad \nabla_{b_1} b_7 = -\frac{1}{2} b_4, \quad \nabla_{b_2} b_1 = -\frac{1}{2} b_5, \quad \nabla_{b_2} b_4 = \frac{1}{2} b_6,$$

$$\nabla_{b_2} b_5 = \tfrac{1}{2} b_1, \ \nabla_{b_2} b_6 = -\tfrac{1}{2} b_4.$$

Let $\xi = \sum a_i b_i$ be a parallel vector field on $\mathbf{37B_1}$. Then for all basis elements, we have $\nabla_{b_i} \xi = 0$.

$$0 = \nabla_{b_1} \xi = \frac{a_2}{2} b_5 + \frac{a_3}{2} b_6 + \frac{a_4}{2} b_7 - \frac{a_5}{2} b_2 - \frac{a_6}{2} b_3 - \frac{a_7}{2} b_4$$

implies $a_2 = a_3 = a_4 = a_5 = a_6 = a_7 = 0$.

$$0 = \nabla_{b_2} \xi$$

gives $a_1 = 0$.

The algebra $\mathbf{37D_1}$:

The non-zero brackets are

$$[b_1, b_2] = b_5, [b_1, b_3] = b_6, [b_1, b_4] = b_7, \ [b_2, b_3] = -b_7, \ [b_2, b_4] = b_6, [b_3, b_4] = -b_5.$$

Some of the nonzero covariant derivatives are:

$$\nabla_{b_1} b_2 = \frac{1}{2} b_5, \quad \nabla_{b_1} b_3 = \frac{1}{2} b_6, \quad \nabla_{b_1} b_4 = \frac{1}{2} b_7, \quad \nabla_{b_1} b_5 = -\frac{1}{2} b_2,$$
$$\nabla_{b_1} b_6 = -\frac{1}{2} b_3, \quad \nabla_{b_1} b_7 = -\frac{1}{2} b_4, \quad \nabla_{b_2} b_1 = -\frac{1}{2} b_5.$$

Let $\xi = \sum a_i b_i$ be a parallel vector field on $\mathbf{37D_1}$. Then for all basis elements, we have $\nabla_{b_i} \xi = 0$.

$$0 = \nabla_{b_1} \xi = \frac{a_2}{2} b_5 + \frac{a_3}{2} b_6 + \frac{a_4}{2} b_7 - \frac{a_5}{2} b_2 - \frac{a_6}{2} b_3 - \frac{a_7}{2} b_4$$

implies $a_2 = a_3 = a_4 = a_5 = a_6 = a_7 = 0$.

$$0 = \nabla_{b_2} \xi$$

gives $a_1 = 0$.

By similar calculations on each of the indecomposable nilpotent Lie algebras over $\mathbb{R}$ in the list of [6], we see that there are no non-zero parallel vector fields on any of the algebras in this list in dimension 7. ■

As an example, we choose one of the algebras in the list of [6] and we investigate the existence of almost cosymplectic and almost α −Sasakian structures on this Lie algebra.

Example Consider the Lie algebra $\mathbf{37A}$ in the list of [6] with upper central series dimension 37. Suppose that (ϕ, ξ, η, g) is an almost contact metric structure on $\mathbf{37A}$. We use the basis $\{b_1, \dots, b_7\}$ of this Lie algebra such that basis elements are g-orthonormal. The non-zero brackets, covariant derivatives are given in the proof of the theorem.

Let us show that there are almost cosymplectic structures on $\mathbf{37A}$. The defining relation of an almost cosymplectic structure is $d\Phi = 0$ and $d\eta = 0$. Since

$$\mathbf{0} = 2d\boldsymbol{\eta}(\boldsymbol{X},\boldsymbol{Y}) = (\nabla_{\boldsymbol{X}}\boldsymbol{\eta})\boldsymbol{Y} - (\nabla_{\boldsymbol{Y}}\boldsymbol{\eta})\boldsymbol{X} = \boldsymbol{g}(\nabla_{\boldsymbol{X}}\boldsymbol{\xi},\boldsymbol{Y}) - \boldsymbol{g}(\nabla_{\boldsymbol{Y}}\boldsymbol{\xi},\boldsymbol{X}),$$

$d\boldsymbol{\eta} = \mathbf{0}$ if and only if the characteristic vector field $\boldsymbol{\xi}$ satisfies

$$\boldsymbol{g}(\nabla_{\boldsymbol{X}}\boldsymbol{\xi},\boldsymbol{Y}) = \boldsymbol{g}(\nabla_{\boldsymbol{Y}}\boldsymbol{\xi},\boldsymbol{X})$$

for all vector fields $\boldsymbol{X},\boldsymbol{Y}$, or equivalently, if and only if

$$\boldsymbol{g}(\nabla_{\boldsymbol{b_i}}\boldsymbol{\xi},\boldsymbol{b_j}) = \boldsymbol{g}(\nabla_{\boldsymbol{b_j}}\boldsymbol{\xi},\boldsymbol{b_i})$$

for all basis elements. Let $\boldsymbol{\xi} = \sum \boldsymbol{a_i}\,\boldsymbol{b_i}$ be the characteristic vector field of an almost cosymplectic structure. Then

$$\boldsymbol{g}\big(\nabla_{\boldsymbol{b_1}}\boldsymbol{\xi},\boldsymbol{b_2}\big) = \boldsymbol{g}\big(\nabla_{\boldsymbol{b_1}}(\boldsymbol{a_1}\boldsymbol{b_1} + \cdots + \boldsymbol{a_7}\boldsymbol{b_7}),\boldsymbol{b_2}\big) = -\frac{\boldsymbol{a_5}}{\mathbf{2}}$$

and

$$\boldsymbol{g}\big(\nabla_{\boldsymbol{e_2}}\boldsymbol{\xi},\boldsymbol{e_1}\big) = \frac{\boldsymbol{a_5}}{\mathbf{2}}$$

implies $\boldsymbol{a_5} = \mathbf{0}$. Similarly checking the conditions

$$\boldsymbol{g}(\nabla_{\boldsymbol{b_i}}\boldsymbol{\xi},\boldsymbol{b_j}) = \boldsymbol{g}(\nabla_{\boldsymbol{b_j}}\boldsymbol{\xi},\boldsymbol{b_i})$$

for all basis elements gives $\boldsymbol{a_6} = \boldsymbol{a_7} = \mathbf{0}$.

Let $\boldsymbol{\Phi} = \sum \boldsymbol{a_{ij}}\boldsymbol{b^{ij}}$, where $\boldsymbol{b^{ij}}$ denotes $\boldsymbol{b^i} \wedge \boldsymbol{b^j}$, and $\boldsymbol{b^i}$ is the dual of the vector field $\boldsymbol{b_i}$ Then

$$\begin{aligned} d\boldsymbol{\Phi} = {} & (\boldsymbol{a_{16}} + \boldsymbol{a_{35}})\boldsymbol{b^{123}} + (\boldsymbol{a_{17}} + \boldsymbol{a_{45}})\boldsymbol{b^{124}} - \boldsymbol{a_{56}}\big(\boldsymbol{b^{126}} - \boldsymbol{b^{235}}\big) - \boldsymbol{a_{57}}\big(\boldsymbol{b^{127}} - \boldsymbol{b^{245}}\big) \\ & + (\boldsymbol{a_{46}} - \boldsymbol{a_{37}})\boldsymbol{b^{234}} - \boldsymbol{a_{67}}(\boldsymbol{b^{237}} - \boldsymbol{b^{246}}). \end{aligned}$$

Thus $d\boldsymbol{\Phi} = \mathbf{0}$ if and only if $\boldsymbol{a_{16}} = -\boldsymbol{a_{35}}$, $\boldsymbol{a_{17}} = -\boldsymbol{a_{45}}$, $\boldsymbol{a_{46}} = \boldsymbol{a_{37}}$ and $\boldsymbol{a_{56}} = \boldsymbol{a_{57}} = \boldsymbol{a_{67}} = \mathbf{0}$. For example, the structure $(\boldsymbol{\phi},\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{g})$, where $\boldsymbol{\xi} = \boldsymbol{e_1}$, $\boldsymbol{\eta} = \boldsymbol{b^1}$, $\boldsymbol{\phi}(\boldsymbol{b_1}) = \mathbf{0}$, $\boldsymbol{\phi}(\boldsymbol{b_2}) = -\boldsymbol{b_5}$, $\boldsymbol{\phi}(\boldsymbol{b_3}) = -\boldsymbol{b_6}$, $\boldsymbol{\phi}(\boldsymbol{b_4}) = -\boldsymbol{b_7}$, $\boldsymbol{\phi}(\boldsymbol{b_5}) = \boldsymbol{b_2}$, $\boldsymbol{\phi}(\boldsymbol{b_6}) = \boldsymbol{b_3}$, $\boldsymbol{\phi}(\boldsymbol{b_7}) = \boldsymbol{b_4}$ is such a structure.

Next we show that there is no almost $\boldsymbol{\alpha}$ −Sasakian structure on $\boldsymbol{37A}$, that is an almost contact metric structure such that $\boldsymbol{\alpha\Phi} = d\boldsymbol{\eta}$, where $\boldsymbol{\alpha}$ is a differentiable function on $\boldsymbol{37A}$. Let $\boldsymbol{\eta} = \boldsymbol{a_1}\boldsymbol{b^1} + \cdots + \boldsymbol{a_7}\boldsymbol{b^7}$. Then

$$d\boldsymbol{\eta} = -\boldsymbol{a_5}\boldsymbol{b^{12}} - \boldsymbol{a_6}\boldsymbol{b^{23}} - \boldsymbol{a_7}\boldsymbol{b^{24}} = \boldsymbol{\alpha\Phi}.$$

In this case, we have $\boldsymbol{\Phi} \wedge \boldsymbol{\Phi} = \mathbf{0}$, which can not be the case, since for an almost contact metric structure in 7-dimensions, we have $\boldsymbol{\eta} \wedge \boldsymbol{\Phi^3} \neq \mathbf{0}$, see [10]

CONFLICT OF INTEREST

The author stated that there are no conflicts of interest regarding the publication of this article.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

EXPLORING IT DECISION MAKERS' VIEWS ON ADOPTION OF CLOUD MANUFACTURING IN TURKEY

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ABSTRACT

Cloud manufacturing has emerged as a breakthrough of IT services, including the internet of things (IoT) and artificial intelligence (AI) for business processes in the manufacturing sector. It has also brought the need to complete the integrated business processes such as an integrated supply chain, inventory management, and production for utilizing this technology. In this context, IT decision-makers attempt to develop a cloud-based manufacturing model for downloading, configuring, and maintaining machinery from cloud providers that enables the top managers just to focus on their product in business. The research aims to build for monitoring the differences between cloud manufacturing adopters and non-adopters to understand the behavioral intention by monitoring the Diffusion of Innovation (DOI) theory and the Technological, Organizational, and Environmental (TOE) theory of cloud manufacturing adoption. An independent t-test sample was used to analyze data. 19 manufacturing cloud adopters and 19 non-cloud adopters were selected to analyze data via SPSS 26.0 in Turkey. The results exhibited that manufacturing cloud adopters and non-cloud adopters considered the same for relative advantage, cost-saving, competitive pressure, and regulatory support. However, they found differences in security concerns, compatibility, complexity, technological readiness, and top management support. The study brought an outlook for understanding the benefits, drawbacks, and hinders of cloud manufacturing of manufacturers. This will enable comprehensive information for cloud providers to offer appropriate integrated software according to manufacturers' needs of the production.

Keywords: Cloud Manufacturing Adoption, IT decision-makers, Independent t-test analysis, DOI theory, TOE theory

1. INTRODUCTION

With Web 3.0 technology, cloud computing has changed the way business model and operation management was operated in the manufacturing sector by the digital transformation [1]. With this technology shift, cloud-based manufacturing was developed to enclose cloud computing, virtualization, and the Internet of things (IoT) for these operations to increase productivity and decrease costs [2]. Along with these benefits, the investment in cloud manufacturing has also been increased recently and in the future. CtrlS [3] underlined that spending on cloud-based manufacturing was $19.1 billion in 2017 and is expected to raise $28.8 billion by 2028. With the cloud manufacturing market growth numerically, it was undoubtedly seen that cloud computing usage was demanded. 88 percent of manufacturing enterprises considered moving to the cloud [3]. Cloud computing was nearly implemented by 66 percent of manufacturing enterprises in practice [4]. 82 percent of manufacturing enterprises applied product lifecycle management (PLM) strategies and applications to shift their real-time business decisions through cloud manufacturing. Thus, the study is required as it contributes to obtaining information from Turkish manufacturers to adopt cloud manufacturing and giving a comprehensive knowledge about the possibility of barriers to cloud manufacturing providers

There have been several definitions of the cloud. The description of the cloud was defined as data, which was stored outside of servers [5]. Hoberg et al. [6] described the cloud as software, which is hosted by the internet. Youseff et al. [7] defined the cloud as the virtualization of computers to utilize manufacturers' operations. Cloud was described as a pay-per-use model of software over the internet

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[8]. Lele [9] defined the cloud as an environment, in which the automated system was built by the external cloud suppliers under service level agreements.

The definitions of cloud manufacturing are varied by distinct scholars. Wu et. al. [10] described cloud manufacturing as a demand-driven manufacturing model to develop flexible solutions for industrial systems. Milisavljevic-Syeda et al. [11] extended the cloud manufacturing definition as utilization of real-time data for contributing real-time supply chain under the internet of things(IoT) enabled quality improvement and robot improvement. Hence, Mukhopadhyay & Mukhopadhyay [12] suggested the term cloud-based manufacturing that has become a basis of Industrial 4.0 development with artificial intelligence (AI) and machine learning to build a continuous improvement frame for sustaining the businesses' existence. There are many benefits of cloud manufacturing, as well as limitations. The benefits of cloud manufacturing were classified into two groups: business and technical. From the business perspective, automated ordering systems mentioned by Forbes [13] were applied to minimize inventory costs. Business intelligence was integrated to apply company-wide intelligence [14]. From the technical perspective, cloud manufacturing served to build elasticity in resource allocation and develop desktop grid applications based on the size and storage of manufacturers [15]. The limitations of cloud manufacturing were lack of control and perceived weaker security [16]. For lack of control, the cloud computing architectural plan for cloud manufacturing adoption was obliged to specify the level of adoption to avoid dependency over cloud manufacturing providers. For perceived weaker security, data owners should have absolute authorization to access data at any time [15]. They should also cooperate with IT auditors to audit the IT assets by specifying control procedures against volatile attacks [17].

There are several studies, in which IT adoption theories were held. Sallehudin et al. [18] proposed a DOI theory to observe the successful implementation of cloud computing adoption from a technical perspective. Alajmi et al. [19] presented an integrated DOI and fit viability model (FVM) to observe the benefits of cloud computing adoption from a manager's perspective. Gutierrez et al. [20] developed a technological, organizational, and environmental (TOE) model to observe the factors influencing cloud computing adoption from an external perspective. There are plenty of studies related to cloud manufacturing adoption in the manufacturing sector. Saleem Al-Shura et al. [21] investigated the important factors in the Pharmaceutical sector in Jordan. Narkhede et al. [22] formed a SWOT analysis for the strategic survival of Indian manufacturing sectors. Oliveira et al. [23] compared manufacturers with the service sector about the necessity of cloud-based service offerings adoption in Portugal. Kyriakou et al. [24] explored the factors affecting cloud computing adoption of glass, ceramic, and cement sectors in France, the UK, Italy, Germany Spain, and Poland. Yassin& Alnidawy [25] specified the adoption requirements of the manufacturing sector in Iraq. Seifu et al. [26] inspected public and private manufacturers in Ethiopia. Goktas& Baysal [27] examined the cloud-based human resource systems in Turkish manufacturers. Narkhede et al. [22] probed the educational sector of India. As a result, there are researches on cloud computing adoption applied IT adoption theories there is no specific study to compare non-cloud manufacturers and cloud manufacturers by applying IT adoption theories such as DOI theory, institution theory, and TOE models for developing countries.

The study has the contribution for cloud manufacturing providers and cloud manufacturing market by analyzing non-cloud manufacturers and cloud manufacturer adopters' intentions over a cloud manufacturing adoption. Since there are no specific studies to compare non-cloud manufacturers and cloud manufacturers applied IT adoption theories, DOI and TOE model was proposed in this study to understand the behavioral differences among non-cloud manufacturers and cloud manufacturers from both technical and external aspects

2. MATERIALS AND METHODS

This study compares and contrasts innovation diffusion factors and TOE factors towards cloud adopters and non-cloud adopters in the manufacturing sector in Turkey. Corresponding research questions are:

1. What are IT decision makers' views about innovation diffusion and TOE factors of cloud adopter manufacturers over non-cloud adopter manufacturers?
2. Are there any significant differences in the views of innovation diffusion and TOE factors of cloud adopter manufacturers over non-cloud adopter manufacturers?

The research design was descriptive and deductive with the independent variable of adopter types (adopter or non-adopter). The independent variables were derived from DOI and TOE theory. The first part of the study consists of eight demographic information of IT decision-makers in terms of gender, education level, working experience, age, market region, cloud application use with numbers, company sizes, and sectors as shown in Table 1. The second part of the study contains DOI and TOE theories questionnaires, including 5 Likert scales ranging from 1 (strongly disagree) to 5 (strongly agree) as shown in Table 2.

Table 1. Demographic information of participants

IT Decision Makers (N=38)	**Variables**	**Frequencies**	**Percentages**
1. Gender	Male	23	60.5%
	Female	15	39.5%
2. Education Level	High School	1	2.6%
	Vocational School	2	5.3%
	Graduate	24	63.2%
	Postgraduate	10	26.3%
	Doctorate	1	2.6%
3. Working Experience	1-3 years	6	15.8%
	4- 7 years	11	28.9%
	8- 10 years	11	28.9%
	11-20 years	7	18.4%
	21 years and above	3	8.0%
4. Age	Age 20-25	0	0%
	Age 26-30	11	28.9%
	Age 31-35	10	26.4%
	Age 36-40	5	13.2%
	Age 41-45	1	2.6%
	Age 46 and above	11	28.9%
5. Market Region	International	23	60.5%
	National	15	39.5%
6. Cloud App with Numbers	1-3 services	13	34.2%
	4-6 services	3	7.9%
	7 and above services	3	10.5 %
	None	19	53.5%
7. Company Size	Micro Manufacturers (1-9)	8	21.1%
	SMEs (10-249)	19	50.0%
	Large Manufacturers	11	28.9%
8. Sectors	Textile	5	13.1%
	Automative	1	2.6%
	Energy	2	5.2%
	Construction	3	7.8%
	Ceramics	2	5.2%
	Pharmaceutical	3	7.8%
	Food	22	57.8%

The data was collected from 38 manufacturing companies. The most frequencies and percentages of IT decision-maker profiles are graduate males aged between 26 and 35, working between 4 and 10 years

in the international and small and medium companies, using between 1 and 3 cloud-based services in the food sector, as illustrated in Table 1. The proportions of the sectors were the food sector by 57.8%, 13.1% by textile sector, construction sector by 7.8%, pharmaceutical sector by 7.8%, energy sector by 5.2%, ceramics sector by 5.2%, and automative sector by 2.6%.

The aim of using an independent t-test is to understand whether relative advantage, cost-saving, security concerns, compatibility and complexity adopted from DOI theory, and technological readiness, top management support, competitive pressure, and regulatory support adopted from TOE theory differed based on cloud adopters and non-cloud adopters.

Here are the null (H0) and the alternate hypothesis (H1) of DOI theory from 'a' to 'e'.

H0a: There is no difference in relative advantage (RA) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1a: There is a difference in relative advantage (RA) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0b: There is no difference in cost-saving (CS) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1b: There is a difference in cost-saving (CS) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0c: There is no difference in security concerns (SC) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1c: There is a difference in security concerns (SC) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0d: There is no difference in compatibility (CO) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1d: There is a difference in compatibility (CO) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0e: There is no difference in complexity (CX) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1e: There is a difference in complexity (CX) between cloud adopter manufacturers and non-cloud adopter manufacturers.

Here are the null (H0) and the alternate hypothesis (H1) of TOE theory from 'f' to 'i'.

H0f: There is no difference in technological readiness (TR) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1f: There is a difference in technological readiness (TR) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0g: There is no difference in top management support (TMS) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1g: There is a difference in top management support (TMS) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0h: There is no difference in competitive pressure (CP) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1h: There is a difference in competitive pressure (CP) between cloud adopter manufacturers and non-cloud adopter manufacturers.

H0i: There is no difference in regulatory support (RS) between cloud adopter manufacturers and non-cloud adopter manufacturers.

And the alternative hypothesis is:

H1i: There is a difference in regulatory support (RS) between cloud adopter manufacturers and non-cloud adopter manufacturers.

The results and discussion of the demographic data, DOI and TOE factors were specified in the following sections.

3. RESULTS

The data is also normally distributed. As it is illustrated in Table 2, the skewness (SK) values and the kurtosis (RKU) values of the range should be between -1 and +1 [28], which all factors were satisfied except the relative advantage factor of cloud manufacturing adopters and the compatibility factor of non-cloud manufacturing adopters. The skewness (SK) values and the kurtosis (RKU) values of the range were between -1.5 and +1.5 [29], which is the relative advantage factor of cloud manufacturing adopters, the security concerns, compatibility, and technology readiness factors of non-cloud manufacturing adopters were satisfied.

An independent-samples t-test was conducted to compare factors of DOI and TOE theory in cloud manufacturing adopters and non-cloud manufacturing adopters. The result was also declared below and presented in Table 2.

Table 2. Mean (M), standard deviations (SD), skewness (SK), and Kurtosis (RKU), and the Results for manufacturing cloud adopters and non-cloud adopters

(N=38)	**MANUFACTURING CLOUD ADOPTERS**				**MANUFACTURING NON-CLOUD ADOPTERS**				**RESULTS**
THEORIES	**M**	**SD**	**SK**	**RKU**	**M**	**SD**	**SK**	**RKU**	
DOI Theory									
RA (Items 1-5)	3.74	0.54	1.06	1.30	3.63	0.66	0.32	-0.08	**H0a Supported**
CS (Items 6-8)	3.56	0.55	0.96	0.80	3.36	0.56	-0.18	0.76	**H0b Supported**
SC (Items 9-11)	2.80	0.50	-0.16	-0.42	3.82	0.86	-0.09	-1.29	**H1c Supported**
CO (Items 12-15)	3.68	0.82	0.32	-0.80	2.86	0.75	-1.20	1.63	**H1d Supported**
CX (Items 16-19)	2.65	0.71	0.44	1.15	3.14	0.62	-0.10	-0.50	**H1e Supported**
TOE Theory									
Technological Context									
TR (Items 20-21)	3.65	0.97	-0.14	-1.02	2.86	0.66	-0.09	-1.37	**H1f Supported**
Organizational Context									
TMS (Items 22-24)	3.78	0.73	0.21	-0.98	2.94	0.65	0.44	-0.25	**H1g Supported**
Environmental Context									
CP (Items 26-28)	2.94	0.80	-0.27	-1.24	2.70	0.73	-0.42	-0.01	**H0h Supported**
RS (Item 28-29)	2.94	0.79	0.65	1.33	2.76	0.51	-0.95	0.85	**H0i Supported**

- RA is found that there is no significant difference between adopters (M = 3.74, SD = 0.54) and non-adopters (M = 3.63, SD = 0.66) with t (36) = -0.586, p = 0.562. **(H0a Supported)**

- CS is found that there is no significant difference between adopters (M = 3.56, SD = 0.55) and non-adopters (M = 3.36, SD = 0.56) with t (36) = -1.061, p = 0.296. **(H0b Supported)**

- SC is found as the significant difference between adopters (M = 2.80, SD = 0.91) and non-adopters (M = 3.82, SD = 0.86) with t (28.883) = 4.444, p = 0.000. **(H1c Supported)**

- CO is found as the significant difference between adopters (M = 3.68, SD = 0.82) and non-adopters (M = 2.86, SD = 0.75) with t (36) = -3.179, p = 0.003. **(H1d Supported)**

- CX is found as the significant difference between adopters (M = 2.65, SD = 0.71) and non-adopters (M = 3.14, SD = 0.62) with t (36) = 2.229 p = 0.032. **(H1e Supported)**

- TR is found as the significant difference between adopters (M = 3.65, SD = 0.97) and non-adopters (M = 2.86, SD = 0.66) with t (36) = -2.923, p = 0.012. **(H1f Supported)**

- TMS is found as the significant difference between adopters (M = 3.78, SD = 0.73) and non-adopters (M = 2.94, SD = 0.65) with t (36) = -3.753, p = 0.000. **(H1g Supported)**

- CP is found that there is no significant difference between adopters (M = 3.78, SD = 0.89) and non-adopters (M = 2.94, SD = 0.85) with t (36) = -0.983, p = 0.332. **(H0h Supported)**

- RS is found that there is no significant difference between adopters (M = 3.78, SD = 0.89) and non-adopters (M = 2.94, SD = 0.85) with t (36) = -0.848, p = 0.403 **(H0i Supported)**

4. DISCUSSION

Cloud manufacturing adoption was at a low level in every sector since only 34.2% of the manufacturers used 1-3 cloud manufacturing services. Adopters related to RA, CS, CP, and RS had also the commonly perceived judgment, whereas non-adopters related to SC, CO, CX, TR, and TMS had different opinions over cloud manufacturing adoption. Amongst the sectors, the highest participants were the food sectors, which affected the results over more agreeing on environmental effects but consider differently over technological and organizational factors. Common and different judgments were declared in the subsections.

4.1. Current Common Views on Cloud Manufacturing Adoption among Manufacturing Adopter and Manufacturing Non-adopters

IT adopters of Manufacturing Adopter and IT adopters of Manufacturing Non-Adopter agreed with each other about RA (H0a), CS (H0b), CP (H0h), and RS(H0i).

For RA, manufacturing cloud manufacturing adopters and non-cloud manufacturing adopters agreed equally that cloud manufacturing adoption finishes specific tasks rapidly, uses business operations easily, improves the quality of operations, offers new opportunities, and increases productivity. Applying the human factor and the automated processes at the right time is important for the process of product design and supply chain to reach customers fast via cloud manufacturing [30]

For CS, manufacturing cloud adopters are considered the same as non-cloud manufacturer adopters about cloud manufacturing adoption that has benefits over adoption costs, decreasing energy costs,

environmental costs, and decreasing maintenance costs. Applying a cost-benefit analysis of production planning, return of investment of supply chain tools, and cloud manufacturing provider selection is significant for manufacturers to specify the invariable costs within a reasonable budget [31].

For CP, manufacturing cloud adopters and manufacturing non-cloud adopters agreed equally because of influencing competition in their industry and their competitors have already started using cloud computing. Application program interface (API), cloud, and artificial intelligence (AI) are the main challenges of cloud manufacturing adoption for the internet & IT systems of manufacturers [32].

For RS, manufacturing cloud adopters admitted equally that there is legal protection in the use of cloud computing and the laws and regulations that exist nowadays are sufficient to protect the use of cloud manufacturing. Because of the absence of the safe harbor agreement in Turkey against Europe and the US for data migration, third-party cloud providers have vulnerable defects for preventing patents, industrial design, and trademarks [33].

4.2. Current Different Views on Cloud Manufacturing Adoption among Manufacturing Adopter and Manufacturing Non-adopters

IT adopters of Manufacturing Adopter and IT adopters of Manufacturing Non-Adopter consider differently about SC (H1c), CO (H1d), CX (H1e), TR (H1f), and TMS (H1g) with the mean differences -1.02, 0.82. -0.49, 0.79, and 0.84, respectively

For SC, the company's data security concerns, customer data security concerns, and concerns about privacy manufacturing of non-cloud adopters in cloud manufacturing were by far higher than the cloud manufacturing adopters. Creating a policy and procedures is important for every step of IT assets such as RFID, QR barcode, and computer-aided manufacturing (CAM) systems, as they can reduce the vulnerability of inside attacks and threats of outside attacks in the supply chain [17]. Computer-assisted audit techniques should be applied by IT auditors to trace bugs, unpermitted entry of networks, and report to the top managers [34].

For CO, cloud adopter manufacturers were much different from non-cloud adopter manufacturers in that they fit the work style of the company, are compatible with business operations, with the company's corporate culture and value system, and with existing hardware and software in the company. Creating education platforms and guidelines is significant to specify the job descriptions for deploying every workers' duties and evolving their qualifications in every workstation of the assembly lines [35]. Audit evidence collection techniques such as interviews and preliminary surveys should be conducted to understand the business risks and the critical processes of business operations [34].

For CX, cloud manufacturing adopters had slightly a high level of mental effort, the advanced skills than non-cloud manufacturing adopters. The data of manufacturing processing planning (MRP), warehouse management, assembly-line monitoring, and customer relationship management should be linked in the centralized database system for gathering the simplicity of manufacturing systems [17]. Business process improvement and business process reengineering should be applied in the short and long term of avoiding complexity by forming project groups from separate business functions, such as marketing, sales, production, and human resources [31]

For TR, cloud manufacturing adopters much more had necessary IT infrastructures and a high level of internet access to implement cloud computing than non-cloud manufacturing adopters. 5G internet is an important basis for increasing broadband data connection and internet bandwidth speed, which it is expected to build in the next years [33]. Fiber buildings should be built for using IT assets effectively for the next decades to build IoT applications with algorithmic artificial intelligence solutions [32].

For TMS cloud manufacturing adopters much more had strong leadership and an ability to take financial and organizational risks than non-cloud manufacturing adopters. Line managers and staff in the workstations should be collaborated to reduce blocking and starving situations against bottleneck issues in the company's operations [35]. Enterprise systems such as Enterprise resource planning (ERP), supply chain management system (SCM), and customer relationship management (CRM) should be well-integrated to report top-level managers as clear spreadsheets to forecast the operating, sales, production, and human resource plan [36].

IT decision-makers should specify hinders, and drawbacks of cloud manufacturing adoption according to their IT assets, policies, procedures, guidelines for the automated and manual processes of their companies' business processes. IT decision-makers should also build a centralized database system for the integration of Application program interface (API), cloud, and artificial intelligence (AI) into their master MRP systems processes to reach customers fast in the market by considering the cost-benefit analysis of the production and supply chain.

5.CONCLUSION

The research contributes to cloud providers for understanding the enthusiasm of non-adopters into two theories: DOI and TOE theory. It also gives the courage of manufacturing non-cloud adopters by acknowledging them of manufacturing cloud adopters' views before cloud manufacturing adoption. The results show that there is a far difference in security concerns, much difference in compatibility, top management support, and technological readiness, and a slight difference in complexity among manufacturing cloud adopters and manufacturing non-cloud adopters, whereas there is not a significant difference in relative advantage, cost-saving, competitive pressure, and regulatory support among manufacturing cloud adopters and manufacturing non-cloud adopters.

Internal factors such as trialability and prior IT experience factors could be applied to examine cloud manufacturing adoption processes from previous experiences. This study will also be extended by monitoring small and medium enterprises (SMEs), large enterprises (LEs), and international companies (IC) for further cloud manufacturing adoption research.

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CONFLICT OF INTEREST

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