Bull. Chem. Soc. Ethiop. **2025**, 39(1), 177-187.
© 2025 Chemical Society of Ethiopia and The Authors
DOI: https://dx.doi.org/10.4314/bcse.v39i1.15

ISSN 1011-3924
Printed in Ethiopia
Online ISSN 1726-801X

ELECTRICAL CONDUCTANCE STUDY OF SCHIFF BASE IN DIFFERENT SOLVENTS AND TEMPERATURES: DFT CALCULATION

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(Received May 8, 2024; Revised September 4, 2024; Accepted September 4, 2024)

ABSTRACT. The electrical conductivities of the N-(2-chlorobenzylidene)benzylamine (NCB) as Schiff bases (SB) compound in water and methanol were studied in different temperatures, the mixtures of methanol and water studied in various percentages of methanol at 298 K. Initially, the relationship between equivalent conductivity and the square root of molar concentration was plotted to find electrolyte types using Kohlrausch equations. The plot indicates that NCB was weakly associated with water, methanol, and mixtures. Lee-Wheaton equation treated the experimental results of symmetrical electrolytes (1:1) to calculate the conductivity confines: equivalent conductance at infinite dilution Λ_o, association constant KA, and the main distance between ions in solution (R) at best-fit values of (σΛ). Thermodynamic quantities for the ion association reaction (ΔGº, ΔHº and ΔSº) have been measured. Also, the theoretical calculation was used to optimize the energy of the molecule in the gas phase then measured many descriptors by using (AM1, PM3) then DFT. In addition, recalculated the optimization energy in water, and methanol. After theoretical calculation and analysis, it was found that the Λ_o value is related to the molecular volume of the system (molecules assembled in the solvent). As the molecular volume increases, the Λ_o value decreases due to association.

KEY WORDS: Schiff bases, Electrical conductivities, Lee-Wheaton equation, Thermodynamic parameter, DFT

INTRODUCTION

In 1864, Hugo Schiff, the German chemist, developed a new organic compound called the Schiff base (SB) (imine), comprised of >C=N-R structure [1, 2]. It's simply synthesized by a condensation reaction between primary amine and aldehyde or a ketone and release water molecule [3], formed water was removed using a molecular sieve [4]. Aromatic (SB) is relatively more stable than aliphatic, since aromatic Schiff bases (SB) have effective conjugation, therefore, stability increased. Because ketone shows higher Steric hindrance than aldehyde, aldehyde reacts faster than ketone in a condensation reaction to produce SB. SB are classified into four main types including bidentate, tridentate, tetra dentate, and polydentate, if they contain additional functional groups such as ($-NH_2$, -OH, or -SH), the resulting ligand can serve as mixed-donor [5].

It's not an exaggeration to describe SB as versatile compounds. SB can form a high-stable complex with almost any metal ions, with the ability to stabilize different metals in different oxidation states [6], therefore, a substantial number of applications of SB complexes including anti-bacterial activity, anti-fungal activity, anti-cancer/tumor activity, anti-microbial activity, anti-oxidant/anti-inflammatory activities [7], corrosion inhibitors, catalysts [8], pigments, polymer stabilizers, clinical and pharmacological features were performed [9].

Through what was mentioned above, it has become interesting to study the electrical properties of these compounds using specific and equivalent conductivity measurements. Using electroanalytical methods for studying electrical properties is very important, due to their high sensitivity, quick analytical response, selective determination, low power-consumption, lower cost, robust, and eco-friendly [10]. Specific and equivalent conductivities measurements can experimentally determine parameters that are suitable to describe the properties of electron transport since these properties mainly depend on the movements of charges or ions present in the system and are influenced by an externally applied electrical field [11].

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In this research, the treatment of experimental data was carried out using Lee-Wheaton equation. Equivalent conductivity at infinite dilution (Λ_o), conductivity parameters, association constant (K_A), the distance between ions in solution (R), and ionic conductivity were also calculated using Lee-Wheaton equation [12]. For monovalent electrolyte solution (1:1), Lee-Wheaton equation will be used [13]:

$$\Lambda = \Lambda_{\circ}[1+C_1(KR)(\epsilon K) + C_2(KR)(\epsilon K)^2+C_3(KR)(\epsilon K)^3] - \frac{PK}{(1+KR)} (1+C_4(KR)(\epsilon K) + [C_5(KR)(\epsilon K)^2 + KR/12] \quad (1)$$

The values of (P, K, E) are:

$$\epsilon = (|Z|^2e^2/DKT) \quad (2)$$

$$K^2 = (8\,\pi\,N^2e|Z|^2C/1000DKT) \quad (3)$$

$$P = (F\,\sigma|Z|/3\,\pi\,\eta) \quad (4)$$

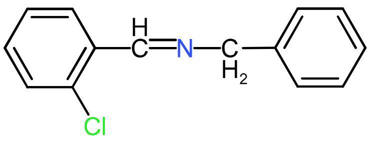
where (Λ) equivalent conductivity, ($\Lambda_{\circ}$) equivalent conductivity at infinite dilution, (F) Faraday's constant, (C) concentration (mol/L), (D) dielectric constant of the solvent, (η) viscosity of the solvent, (σ) conversion factor (Volt-electrostatic) and (R) is the main distance between positive and negative ions.

In daily life, theoretical chemistry is extremely important. It would be impossible to create any medications without the sophisticated research conducted by theoretical chemists. Furthermore, the way our bodies are constructed means that the body can only absorb and use the left-handed version of amino acids [14]. Different approaches are used in theoretical chemistry, including semi-empirical, ab initio, and density functional theory (DFT). In physics, chemistry, and materials science, DFT—a theory of correlated many-body systems—is frequently used to understand and forecast the characteristics and behavior of these systems. It also can estimate the electronic structure of the many-electron system from atoms, molecular, to condensed matter, where the properties of a many-electron system can be expressed as functional of the spatially dependent electron density [15]. The main objective of this work is to investigate computationally, in gas and aqueous phases, using DFT at B3LYP/6-31G$^{(++)}$ level of theory, the intrinsic electronic properties of the structure of the compounds [16].

EXPERIMENTAL

Conductivity analysis

The conductance of N-(2-chlorobenzylidene)benzylamine (NCB) which was previously prepared and identified [17], was measured in water and methanol at temperatures (293 - 313) K at 5 K intervals and (Methanol-Water) mixture in different proportions (10%, 20%, 30%, 40% and 50%) at 298 K.



N-(2-Chlorobenzylidene)benzylamine

The solution was prepared at a normality of ($N = 10^{-4}$), by dissolving (0.00022 g) in a 10 mL of selected solvent. Using a water-circulating ultra-thermostat, the temperature of the conductance cell and its contents was kept at a constant temperature, and the conductance of solvent was measured and recorded before the addition of solution, for more accurate results, correction was made for the specific conductance of the solvents used by subtracting the specific conductivity of the solvents from those of the solute. The cell was washed with water and then dried in the oven. Afterward, the cell and its contents were weighed. The sample was injected into the cell using a plastic syringe, and it was weighed before and after each addition, generally 16 additions (0.1 mL in each addition), magnetic stirrer was used to homogenize the solution, and the conductivity was measured. After that, the cell and its contents were reweighed.

Conductance measurements were carried out on Professional Benchtop Conductivity meter BC3020 with resolution 0.01 µS and accuracy ± 0.01 $\mu S.cm^{-1}$ and the cell constant was 1 cm^{-1}. The conductivity meter used is robust enough to depend on, allowing us to study the electrolyte solution in dilute concentrations. The most important factor for obtaining good conductance results is mainly associated with the preparation of the solution, manipulation, and apparatus cleanliness.

Computational details

Theoretical measurements were carried out using Chemoffice (v16.0.1.4) and Gaussian 0.9 installed on (hp EliteBook x360 1030 G2) with (2.80 GHz). The first estimation of the structural geometry of the compound [N-(2-chlorobenzylidene)benzylamine] was obtained using molecular mechanics (MM2 and MD) and further geometry optimization using AM1, PM3, HF, and finally, DFT optimization and then calculated many descriptors [18].

RESULTS AND DISCUSSION

Conductivity analysis

Equivalent conductivities of NCB were calculated in the temperature range of 293 – 313 K. In all cases, there was a gradual increase in equivalent conductivity (Λ) with increasing temperature, which indicates that the compound lies in the range of semiconductors. Equivalent conductivities concentration values are listed in Tables 1-3.

Table 1. Molar concentration, and equivalent conductance of NCB at 293 to 313 K in methanol.

Conc. (mol/L) $*10^{-6}$	√Conc. (mol/L) $*10^{-3}$	Λ (Ω^{-1}. $equiv^{-1}$. cm^2) at 293 K	Λ (Ω^{-1}.$equiv^{-1}$. cm^2) at 298 K	Λ (Ω^{-1}.$equiv^{-1}$. cm^2) at 303 K	Λ (Ω^{-1}.$equiv^{-1}$. cm^2) at 308 K	Λ (Ω^{-1}.$equiv^{-1}$. cm^2) at 313 K
0.5394	0.7344	39.7726	58.0750	83.4176	94.9527	113.3971
1.0214	1.0106	29.5592	39.9627	58.7410	69.1198	78.3427
1.4857	1.2189	18.6201	33.3624	50.4806	60.8366	66.6757
1.9486	1.3959	17.2593	30.1788	46.1864	56.4901	60.5338
2.4391	1.5617	13.9505	28.5337	43.0473	53.5322	56.8352
2.9061	1.7047	13.3599	27.4907	41.2912	51.8172	54.4641
3.3668	1.8349	11.4583	26.5433	40.0965	50.6525	53.1827
3.8036	1.9503	11.4258	26.1292	39.4354	49.3573	52.1363
4.2703	2.0664	11.2641	25.9312	38.6387	48.7271	51.3951
4.8616	2.2049	11.1418	24.6246	37.0244	46.3757	48.1147
5.3322	2.3091	11.0352	23.2883	35.6321	44.5932	46.5723
5.7642	2.4008	10.2288	22.3820	34.6966	43.7623	45.5812
6.2062	2.4912	9.45902	20.9128	33.8370	43.8867	44.8972
6.6050	2.5700	9.50055	20.2595	33.3076	43.0915	43.5664
7.0765	2.6601	9.01654	19.7312	32.5018	42.5595	42.1838
7.5868	2.7544	8.43819	18.8814	31.6339	40.8393	40.3742

Table 2. Molar concentration, and Equivalent conductance of NCB at 293 to 313 K in water.

Conc. (mol/L) $*10^{-6}$	√Conc. (mol/L) $*10^{-3}$	Λ (Ω^{-1}.equiv^{-1}. cm^2) at 293 K	Λ(Ω^{-1}. equiv^{-1}. cm^2) at 298 K	Λ (Ω^{-1}.equiv^{-1}. cm^2) at 303 K	Λ(Ω^{-1}.equiv^{-1}. cm^2) at 308 K	Λ (Ω^{-1}.equiv^{-1}. cm^2) at 313 K
0.56	0.7536	35.2128	57.7717	66.1833	92.1540	133.659
1.04	1.0184	28.9256	40.6874	47.6591	70.9140	88.7189
1.49	1.2212	20.1148	34.3121	43.3209	60.0939	72.7968
1.95	1.3964	17.9473	31.3187	40.0674	56.6811	66.5311
2.38	1.5423	14.7135	29.0835	38.9944	53.7414	62.5661
2.84	1.6843	14.0992	28.4317	37.9772	51.9056	58.9740
3.24	1.8011	12.3303	27.5546	37.4696	51.3208	57.7419
3.69	1.9221	12.1794	24.0745	37.0138	50.5362	56.2072
4.11	2.0268	12.1716	23.2296	36.7835	50.0001	55.1280
4.66	2.1580	11.8100	23.2060	35.3467	47.2341	53.3614
5.15	2.2685	11.6592	22.2707	34.2005	45.5324	51.8296
5.63	2.3729	10.6555	21.5703	33.2281	44.7175	50.6745
6.03	2.4564	9.9434	20.0989	32.5679	44.7469	49.5447
6.46	2.5408	10.0680	19.5947	31.9423	44.1135	47.7654
6.83	2.6135	9.5159	18.8707	31.3571	43.6381	46.3268
7.38	2.7160	8.8111	18.0907	30.3029	41.8353	44.3497

Table 3. Molar concentration, and Equivalent conductance of NCB in different percentages of methanol in water mixture at 298 K.

Conc. (mol/L) $*10^{-6}$	√Conc. (mol/L) $*10^{-3}$	Λ (Ω^{-1}.equiv^{-1}. cm^2) at 10%	Λ (Ω^{-1}.equiv^{-1} .cm^2) at 20%	Λ (Ω^{-1}.equiv^{-1} .cm^2) at 30%	Λ (Ω^{-1}.equiv^{-1} .cm^2) at 40%	Λ (Ω^{-1}.equiv^{-1} .cm^2) at 50%
0.4220	0.6496	271.3508	233.0526	175.2095	145.3993	130.3013
0.7722	0.8787	106.6203	110.0598	96.0273	87.4359	77.6957
1.1457	1.0703	69.8883	78.0768	74.6852	64.8056	56.7318
1.5232	1.2341	56.1257	62.1079	60.8521	57.4396	49.2385
1.9001	1.3784	48.2806	50.7705	54.8179	52.1473	42.1026
2.2400	1.4966	43.8565	42.4860	49.4811	47.5677	37.9449
2.6000	1.6124	41.4412	38.8679	46.4323	43.7434	36.5378
2.9416	1.7151	39.0127	35.7676	43.2802	43.1770	35.6938
3.3033	1.8175	37.5078	33.8194	42.1524	40.8192	33.2995
3.7775	1.9435	35.6331	30.4736	40.5486	38.4213	31.7664
4.1394	2.0345	34.5062	30.8776	40.2647	38.2883	32.6130
4.4902	2.1190	33.5930	28.4770	39.1223	37.5831	31.1787
4.8677	2.2062	32.9014	27.2073	36.9638	37.9223	29.7880
5.1817	2.2763	31.5725	26.2563	35.8706	35.9183	28.9475
5.5129	2.3479	30.4684	25.2461	33.7205	34.2966	28.1154
5.9290	2.4349	29.2640	24.5772	33.1450	32.8112	26.1427

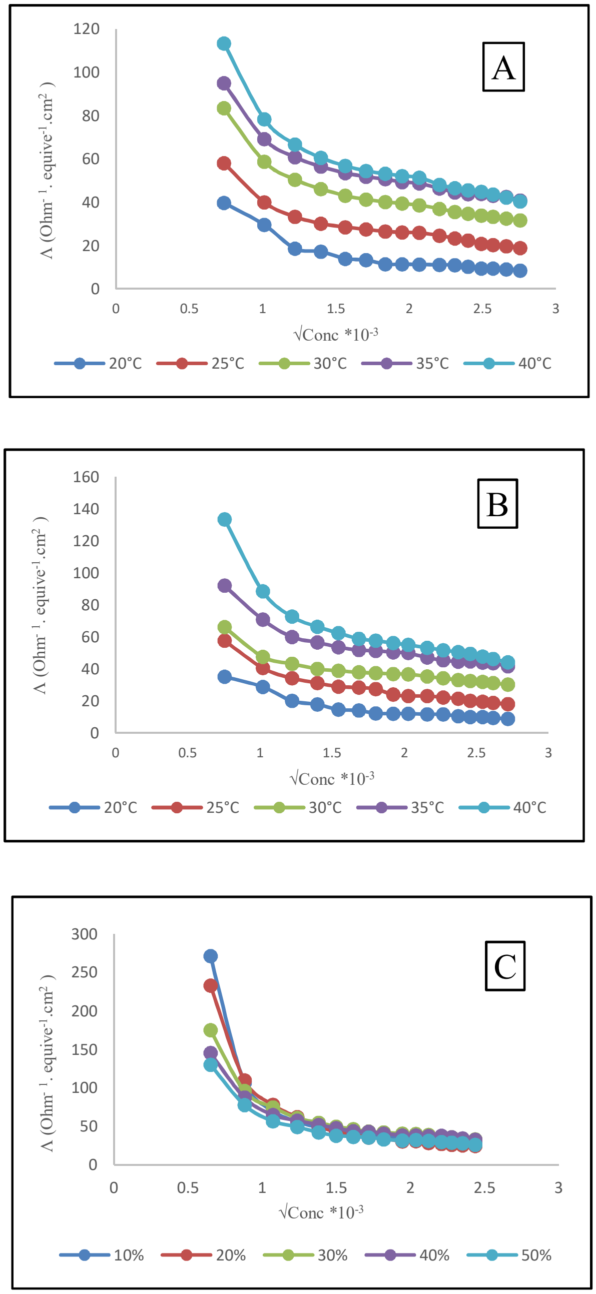


Figure 1. Equivalent conductivities (Λ) of (NCB) as a function of √Conc. in (A) in methanol, (B) in water, and (C) in a water-methanol mixture.

According to these values of Λ, the compound has a positive temperature coefficient, which implies that for a given concentration, the conductivity improves dramatically at higher temperatures. This increase starts when the charge carriers can accelerate due to their increased energy. Additionally, as the temperature rises, the charge carriers' mobility increases [19].

Then the calculation of thermodynamic parameters (ΔG, ΔH and ΔS) was performed using thev Van't-Hoff equation by plotting the relationship of $\ln K_A$ against 1/T [20].

$$lnK_A = -\frac{\Delta H}{RT} + C \tag{5}$$

It gives a straight line of complex solutions, and ΔG calculated by equation:

$$\Delta G = -RTlnK_A \tag{6}$$

And entropy values were calculated by:

$$\Delta G = \Delta H\text{-}T\ \Delta S \tag{7}$$

Table 4. Values of K_A, Λ_o, R, and δΛ for NCB calculated in different solvents.

In methanol				
T(K)	K_A	Λ_o (Ω^{-1}.equiv^{-1}.cm^2)	R (A°)	δΛ
293	1268828	34.827	1	0.0311
298	2153161	87.158	1	0.0183
303	3227729	130.376	1.5	0.0219
308	4590814	103.879	1	0.0350
313	5273365	175.667	1.1	0.0325
In water				
T(K)	K_A	Λ_o (Ω^{-1}.equiv^{-1}.cm^2)	R (A°)	δΛ
293	9855615	159.869	1.5	0.0140
298	11406148	248.285	1.5	0.0196
303	11625529	305.151	1.3	0.0379
308	13512179	307.158	1	0.0406
313	16653513	488.575	1.7	0.0493

In (methanol-water) mixture					
T(K)	%	K_A	Λ_o (Ω^{-1}.equiv^{-1}.cm^2)	R (A°)	δΛ
298	10	3288911	212.534	1	0.4220
	20	8045248	336.974	1	0.4083
	30	12299094	409.156	1	0.3221
	40	2701939	167.834	1	0.1541
	50	1402655	18.439	1	0.1904

The positive values of ΔH, indicating the enthalpy of association, suggest that specific short-range interactions like hydrogen bonding are responsible for this phenomenon. On the other hand, ΔG, the Gibbs free energy, exhibits negative values that vary depending on the type of ions involved, suggesting that the ionic aggregation process happened spontaneously in both water and methanol. While the small positive values of ΔS are a consequence of the negative ΔH values, which lead to the system becoming more ordered due to the influence of solvation and the columbic effect in a continuous medium.

Table 5. Thermodynamic parameters for NCB in different solvents a temperatures.

In methanol					
T(K)	1/T *1000	LnK_A	ΔG (kJ.mol^{-1})	ΔS (J.mol^{-1}.K^{-1})	ΔH (kJ.mol^{-1})
293	3.4129	14.0536	-34.2346	305.1977	55.1883
298	3.3557	14.5824	-36.1290	306.4342	
303	3.3003	14.9872	-37.7551	306.7440	
308	3.2467	15.3395	-39.2802	306.7160	
313	3.1948	15.4781	-40.2785	305.0061	

In water					
T(K)	1/T *1000	LnK_A	ΔG (kJ.mol^{-1})	ΔS (J.mol^{-1}.K^{-1})	ΔH (kJ.mol^{-1})
293	3.4129	16.1035	-39.2282	197.0770	18.5152
298	3.3557	16.2496	-40.2597	197.2315	
303	3.3003	16.2687	-40.9832	196.3646	
308	3.2467	16.4191	-42.0445	196.6229	
313	3.1948	16.6281	-43.2710	197.4005	

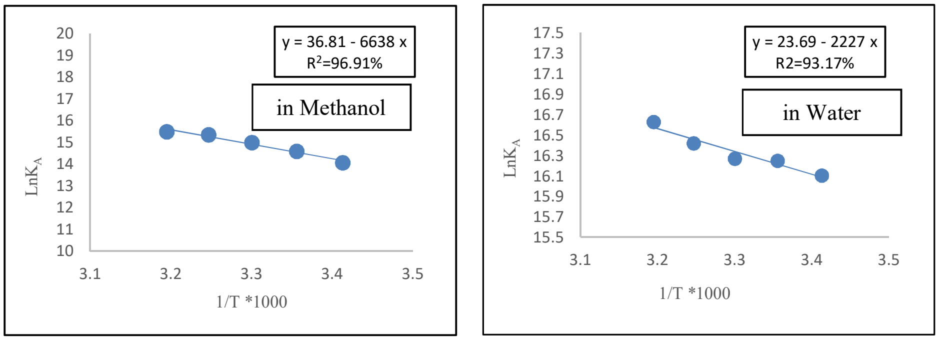


Figure 2. The relation between LnK_A and 1/T for (NCB) calculated in different solvents at (293-313 K).

Walden product ($\eta_o\Lambda_o$)

The Walden Product is calculated by multiplying the viscosity (η_o) and the conductivity at infinite dilution of a solution (Λ_o), which helps in determining the water-structuring activity of the solute. The rise in alcohol percentage leads to a corresponding increase in viscosity due to the molecular interactions between alcohol and water molecules. These interactions have a positive impact on the ($\eta_o\Lambda_o$), causing it to increase. However, they also have a slight effect on the equivalent conductivity value at infinite dilution. As molecular interactions intensify, the number of ionic groups increases, resulting in decreased conductivity. Consequently, when the alcohol percentage reaches 30%, we observe the highest values for the equivalent conductivity at infinite dilution and the ($\eta_o\Lambda_o$).

Table 6. Relation between Walden product ($\eta_o\Lambda_o$) and percentage of methanol in water mixture at 298 K.

Percentage %	η_o	Λ_o (Ω^{-1}. equive^{-1}.cm^2)	$\eta_o\Lambda_o$
10%	0.0013	212.534	0.2912
20%	0.0018	336.974	0.6153
30%	0.0022	409.156	0.9334
40%	0.0027	167.834	0.4593
50%	0.0031	18.439	0.0588

Theoretical results

The DFT/B3LYP/6-31G$^{(+,+)}$ computational level was used to optimize the molecular geometry structure of the compound. Some structural parameters of the optimized molecular geometry were summarized in Table 6. The optimum geometrical form of NCB molecule in different solvents, as the COSMO model is shown in Figure 3.

The fourth approach of calculation was applied to study the energy of the molecule in the gas phase then was recalculation on the solvents (water and methanol) by using B3LYP functional in DFT at 6-31G^{++} CPCM type as shown in Table 7. Descriptors as shown in Table 7 for chemical reactivity calculated by the DFT include total energy E, chemical hardness, electronic chemical potential (μ), and electrophilicity (ω). Chemical hardness measures the system's reactivity and stability by measuring the system's resistance to changes in electron distribution or transfer of charge. It is measured by the difference between HOMO and LUMO, based on the molecular orbitals. At the same time, electrochemical potential is a negative value of the electronegativities of a molecule. On the other hand, electrophilicity (ω) is the tendency to escape from the equilibrium system [21]. Polarizability is obtained by analytical differentiation of a dipole moment related to the electric field, all of these descriptors were calculated according to the equations 8, 9, and 103.

$$\eta = (\varepsilon LUMO - \varepsilon HOMO)/2 \tag{8}$$

$$\mu = (\varepsilon LUMO + \varepsilon HOMO)/2 \tag{9}$$

$$\omega = \mu^2/\,2\eta \tag{10}$$

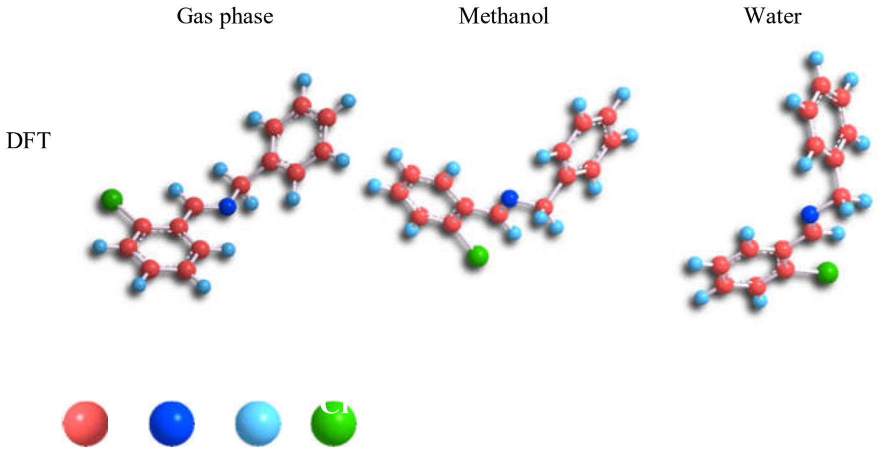


Figure 3. The final geometrical form of NCB molecule in different solvents as the COSMO model.

Table 7 reports the calculated new parameters to describe the molecule in solvents. We can see the differences between many values as changes in the solvent so it will lead to knowing that the physical properties of the solvent were affected by the parameters. The more important parameter that affected the molecule and its conductivity is the change in the solvent, this can be identified this change from the differences between the descriptors like Connolly values especially Connolly Solvent Excluded Volume which refers to the volume of space bounded by the solvent accessible molecular surface [22]. In addition, the value of polarization: polarizability (and hyperpolarizability) provides information about the distribution of electrons based on the presence of an applied electric field. In general, molecules with more delocalized electrons have higher polarizability values. There are many factors affecting the degree of Ionization: Nature of electrolyte: Weak electrolyte dissociates less and strong electrolyte dissociates more. Nature of the solvent: The ionizing power of the solvent depends upon its dielectric constant. Temperature: Effects K value as ($K_w \propto T$) [23]. Then we notice this reflected in the equivalent conductivity values upon infinite dilution, as its value in water is higher than in methanol because of the molecular volume of each solvent.

Table 7. Global chemical reactivity indices of the compound in different systems.

Descriptors	Gas	Water	Methanol
ƐHOMO (eV)	-0.2655	-0.2631	-0.2600
ƐLUMO (eV)	-0.0532	-0.0599	-0.0510
GAP (Δε) (ev)	0.2122	0.2032	0.2089
Ionization potential (I)	0.2655	0.2631	0.2600
Electronic affinity (A)	0.0532	0.0599	0.0510
Hardness (Ƞ)	0.1061	0.1016	0.1044
Chemical potential (μ)	-0.1593	-0.1615	-0.1555
Electrophilicity (ω)	0.1196	0.1284	0.1158
Connolly solvent excluded volume ($Å^3$)	186.546	187.65	187.36
Number of H-bond acceptors	1	1	1
Number of H-bond donors	0	0	0
Ovality	1.4645894713307	1.46168880674292	1.46180322663155
Connolly accessible area ($Å^2$)	449.936	454.063	454.011
Connolly molecular area ($Å^2$)	231.237	231.454	231.468
Dipole (Debye)	1.293	1.2543	1.2543
Molecular volume ($Bohr^{**3}$/mol	1881.957	2064.03	1952.322
RMS force (kcal/mol)	4.1622	4.2837	4.2828
SCF energy (kcal/mol)	-659396.47	-659395.97	-659395.99
Entropy (cal/mol-Kelvin)	108.262	108.226	108.231
Molecular mass (au)	229.06583	229.06583	229.06583
Thermodynamic energy (kcal/mol)	157.243	157.187	157.189
Zero-point energy (kcal/mol)	149.958953	149.906242	149.908752
Principal mment	517.645 2574.802 2931.661	536.090 2543.220 2836.271	536.350 2541.979 2836.282
Polarizability	449.936	454.063	454.011
Molecular topology descriptors			
Balaban index	91409	91409	91409
Cluster count	16	16	16
Polar surface area ($Å^2$)	12.36	12.36	12.36

Num rotatable bonds	3 Bond(s)	3 Bond(s)	3 Bond(s)
Radius	5 Atom(s)	5 Atom(s)	5 Atom(s)
Shape attribute	14.0625	14.0625	14.0625
Topological diameter	10 Bond(s)	10 Bond(s)	10 Bond(s)
Total connectivity	0.003007032652	0.003007032652	0.003007032652
Wiener index	508	508	508

CONCLUSION

In this research, the electrical conductivity of compound [N-(2-chlorobenzylidene)benzylamine] in water and methanol was studied separately at different temperatures within the range of 290-313 K, and the conductivity was also studied in a mixture of the previous two solvents with mixing ratios ranging from 10-50%. By interpreting the results of conductivity and its relationship with concentration through the Kohlrausch equation, it was found that the compound behaves like a weak electrolyte. By analyzing the results in the Lee-Wheaton equation and introducing the physical properties of the solvents used, the equivalent conductivity at infinite dilution, the value of the ionic group constant, and the distance between the ions were obtained.

This behavior was studied at different temperatures to calculate the thermodynamic constants x, y, and K. It is shown that the positive value of the enthalpy indicates that the decomposition was endothermic. The values of ΔG (Gibbs free energy) have negative values that depend on the type of ions and agree with the relationship, which means that the reaction was spontaneous towards the association. The values of ΔS were positive, which leads to the arrangement of the system as a result of association under the melting effect and Coulombic effect in spontaneous continuous media.

The compound was studied using DFT computational programs, and by studying the molar volume of the compound, varies with the solvent, because the molecular volume of compounds in each solvent, which depended on the solvent molecule and its interactions with compound, and other physical properties of solvents. We notice that in the gas phase, it is smaller than in the rest of the systems and larger in the water system, as a result of the effect of the polarity of the solvent on the molecule.

ACKNOWLEDGEMENT

The authors thank the Chemistry Department in the College of Science, University of Mosul, Mosul, Iraq for providing facilities and equipment.

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