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Conductivity Measurements, Thermodynamic Calculations and Theoretical Calculations of N-(2-chlorobenzylidene)-4-picolylamine in Different Solvents and Temperatures.

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Article Informations

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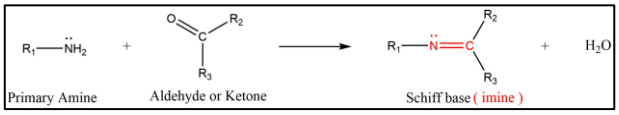
A B S T R A C T

The Electrical conductivity of N-(2-ChloroBenzylidene)-4-picolylamine was benchmarked in different solvents including water & methanol at temperature range of (293-313K) at 5K intervals, and in (Methanol-Water) mixture at 298K in different percentage (10%, 20%, 30%, 40% and 50%). Then plotting the relation between equivalent conductivity (Λ) and square root of molar conc. ($\sqrt{}$Conc.). By using Kohlrausch equation the plot shows that the Schiff base compound act as weak electrolyte, i.e., weak association in water, methanol and (Methanol-Water) mixture. Then applying (Lee-Wheaton) equation for symmetrical electrolyte (1:1) to calculate different thermodynamic parameters including: Association constant (KA), equivalent conductivity at infinite dilution (Λ_o), main distance between ions (R), and Standard deviation ($\sigma\Lambda$). The values of (ΔH, ΔH, ΔS) were measured utilizing (Van't-Hoff) equation. The final step including theoretical calculations to optimize the molecular energy of the compound and measuring different parameters in gas phase, water and methanol using (AM1, PM3) , HF, and DFT/B3LYP/6-31G.

Introduction

Electrical conductivity (EC) is an intrinsic property of materials and is independent of their geometry. The (EC) of liquids is directly proportional to the temperature as the motion of ions increases. The (SI) unit of (EC) is Siemens per centimeter ($S.cm^{-1}$). Substances are classified into three classes, (conductors, semiconductors and insulators) [1]. The study of electrochemistry is based on the movements of electrons in a reduction or oxidation reaction at the surface of the electrode. The analyte is reduced or oxidized at a specific potential, and the amount of current measured is directly proportional to the concentration of the analyte [2].

Schiff Base (SB) is considered one of the most widely used ligands, that's of course, because they are easily formed and their versatility. The formation of (SB) is simple, by condensation reaction between carbonyl compound with a primary amine [3]. (SB) plays important roles especially in coordination chemistry, with the ability to stabilize metal complexes with different oxidation states, (SB) ligands have different types of donors including nitrogen (N), oxygen (O) and sulfur (S) [4]. In recent research, the researchers have confirmed that the presence of azo-methine group (-N=CH-) in (SB) compounds is the main reason for biological properties such as anti-cancer, anti-inflammatory, anti-fungal, anti-microbial, anti-viral, other applications such as corrosion inhibitors, anti-oxidant, pigments, etc. [5].



Scheme 1. Synthesis of Schiff Base.

In this research, the experimental data were treated using (Lee-Wheaton) equation for symmetrical electrolytes (1:1) of Schiff base (SB) in different solvents water, methanol at a temperature range of (293°K-313°K) and (methanol- water) mixture at different percentages at (298°K).

The Kohlrausch bridge, which he adapted from the Wheatstone bridge, is a sufficiently well-established method for measuring common electrolyte solutions and is used in conductivity measurements [6]. The theory of dilute solutions, which describes the reduction in conductivity owing to ion-pair formation, has been extended to the conductivity of concentrated aqueous electrolyte solutions, which has been the subject of increased research in recent years. Conversely, numerous researchers, such as Angell, Watanabe, and others, have examined ionic conductivity not only in concentrated electrolyte solutions but also in molten salts, ionic liquids, and gel electrolytes from the perspective that ionic interactions affect physical properties since the Walden rule was proposed for the correlation between viscosity and conductivity of viscous electrolyte solutions [7].

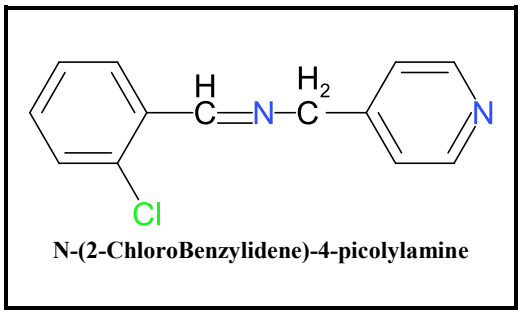
Density functional theory is the technique that can be used extensively for "ab-initio" estimations of the different moieties belonging to organic to inorganic in nature [8]. Due to lower computational cost, and having favourable accuracy, DFT is a definitive technique in most of the branches of material science and chemistry [9]. Complications of electronic structure in a dazzling diversity of fields are directly being tackled. over the last 20 years, DFT has become an excessively used device in most of the chemistry branches [10].

Density functional theory (DFT) has become established as an indispensable tool for investigating aqueous systems of all kinds, including those important in chemistry, surface science, biology, and the earth sciences [11].

2. Experimental

2.1 Conductivity analysis:

The (EC) of N-(2-ChloroBenzylidene)-4-picolylamine was measured in different solvents including water, methanol at a temperature range of (293k-313K), and in (methanol-water) mixture at (298K) in different percentages (10%, 20%, 30%, 40% and 50%).



N-(2-ChloroBenzylidene)-4-picolylamine

According to the molecular weight of the compound, the preparation of the sample solution was performed by dissolving (0.0023g) of the compound in (10ml) volumetric flask using different solvents [water, methanol and (Methanol-Water) mixture], and the volumetric flask was weighted empty and with the sample solution. Then the solution was diluted to the normality of (N=10-4) using dilution law (also in a 10ml volumetric flask). The conductance cell was washed with conductance water and dried, then weighted empty. Then fill the conductance cell with (20ml) of the solvent used. Using water-bath (HAAKE NK22 Refrigerated Circulator Bath) to keep the temperature of the conductance cell and its content at a constant degree. The sample was injected into the conductance cell using a plastic syringe, by injecting (0.1ml) for each reading (16 readings). A magnetic stirrer was used to keep the sample solution and the solvent inside the conductance cell homogenized. After completing all (16 readings), the cell and its content are weighted again and record.

2.2 Computational Details:

Theoretical calculations were performed using (Gaussian 0.9) and (Chem Office 16) installed on HP-EliteBook 1030 with a 2.8 GHz Intel processor. The first step involves geometry optimization of the molecular system using molecular mechanism (MM2 & MD), Then calculating different parameters using (DFT/B3LYP/6-31G) [12].

3. Results & Discussion

3.1 Conductivity Analysis:

The interpretation of conductance data may be done using the Lee-Wheaton equation. The full analysis of mixed symmetrical and asymmetrical electrolytes at various temperatures is done using this equation. When the positive ion is represented by (M+) and the negative ion by (X-) when using the equation for these solutions, the electrical conductivity of the solution of [N-(2-ChloroBenzylidene)-4-picolylamine] was studied in conductivity water & methanol. The solution promised symmetrical electrolytes of type (1:1).

$$M^{+}_{aq.} + X^{-}_{aq.} \xleftrightarrow{Ka} (M_{.aq}{}^{+n}\,X)$$

Ka: association constant

Measuring conductivity is one of the physical characteristics through which the behavior of compounds in different solvents can be explained. We notice that the equivalent conductivity values upon infinite dilution in water and methanol increase with increasing temperatures at the same concentration and decrease with increasing concentration. After measuring electrical conductivity in the solution at all temperatures and in all solvents, this relationship has proven that the solution exhibits weak electrolyte behavior. It belongs to the class of symmetrical (1:1) electrolytes. Figures 1, 2, and 3 as well as tables demonstrate that [N-(2-ChloroBenzylidene)-4-picolylamine] behavior [13].

Table (1): Molar concentration, and Equivalent conductance of [N-(2-ChloroBenzylidene)-4-picolylamine] at (293 to 313 K) in methanol.

Conc. (Mol/lit.) $*10^{-6}$	**√Conc.** (Mol/lit.) $*10^{-3}$	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 293°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 298°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 303°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 308°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 313°k
0.5436	0.7373	83.6467	125.4351	138.4906	161.6952	202.3434
1.0481	1.0238	58.5973	79.0414	95.3038	107.0806	133.5656
1.5325	1.2379	47.4464	66.3633	81.0586	88.7139	110.9272
1.9474	1.3955	40.9793	57.8892	71.9207	81.1740	102.6977
2.4161	1.5543	37.3382	53.4968	65.0138	75.4553	95.1925
2.8667	1.6931	34.9123	48.9026	64.7653	72.1777	90.6940
3.3378	1.8269	34.5450	46.9672	61.5387	69.8671	86.8821
3.7727	1.9423	33.3702	45.7027	59.4023	68.7887	84.8197
4.2153	2.0531	32.1309	45.4016	60.0963	66.4726	83.0301
4.7971	2.1902	32.4709	43.3350	59.6869	64.4609	79.2136
5.3364	2.3100	31.4443	42.2812	59.0561	62.7186	76.8302
5.7671	2.4014	30.8619	41.8743	57.5745	61.6405	76.2937
6.1992	2.4898	29.4029	40.1441	55.5873	60.4305	75.8152
6.6066	2.5703	28.3257	39.1616	54.1487	59.2985	75.6817
7.0581	2.6567	27.2047	38.6904	52.7757	58.5177	75.0910
7.5669	2.7508	26.1218	37.7237	51.8191	57.3962	74.0061

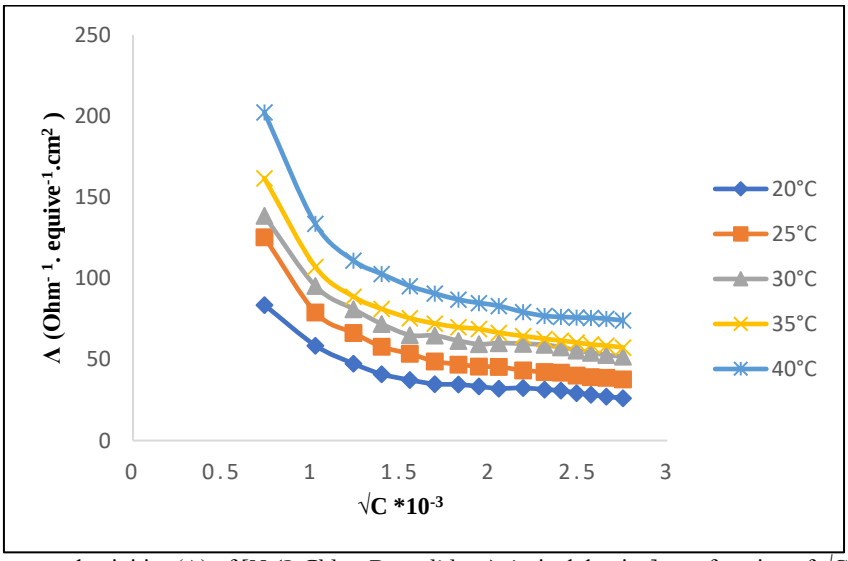


Figure 1. Equivalent conductivities (Λ) of [N-(2-ChloroBenzylidene)-4-picolylamine] as a function of √Conc. at a temperature of (293° to 313°K) in methanol.

Table (2): Molar concentration, and Equivalent conductance of [N-(2-ChloroBenzylidene)-4-picolylamine] at (293 to 313 K) in water.

Conc. (Mol/lit.) $*10^{-6}$	**√Conc.** (Mol/lit.) $*10^{-3}$	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 293°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 298°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 303°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 308°k	**Λ** (Ω^{-1}. equive^{-1}.cm^2) at 313°k
0.5021	0.7086	69.6996	82.4929	131.9804	164.9326	235.7618
1.0159	1.0079	49.2138	59.4534	92.06033	114.2473	158.2819
1.4912	1.2211	43.5871	54.3458	78.0869	97.1235	133.3026
1.9614	1.4005	40.7862	51.5642	72.0947	88.2604	122.7064
2.4208	1.5559	39.2425	50.3289	68.4532	83.3006	115.1431
2.8768	1.6961	38.2367	48.6802	66.1228	80.1866	110.5747
3.3312	1.8251	37.5231	48.3936	64.6448	78.0589	108.1674
3.7636	1.9400	37.1975	47.5643	63.2226	76.7276	107.5808
4.1944	2.0480	36.9535	47.1740	62.5294	75.4474	103.4618
4.6800	2.1633	36.3246	45.1269	60.0164	73.9289	99.1848
5.1701	2.2737	35.7823	45.1728	59.1750	72.9520	96.6949
5.6093	2.3684	35.6546	45.1831	59.0730	72.4065	95.7263
6.0462	2.4589	35.5592	44.6467	58.2233	71.4934	94.5765
6.4900	2.5475	35.4387	43.7213	57.3827	70.5011	93.5997
6.9121	2.6290	34.7215	43.2529	56.5602	69.7485	92.0894
7.5292	2.7439	33.2038	41.8040	55.6011	67.2666	89.3058

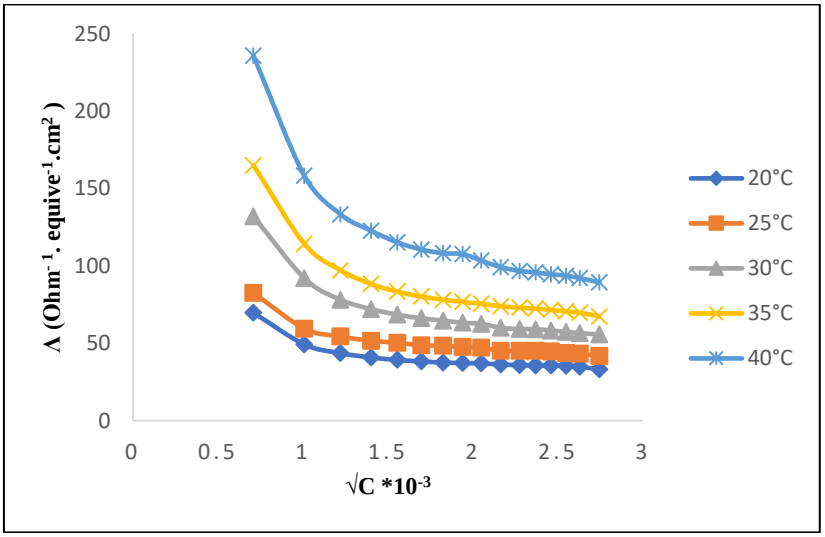


Figure 2. Equivalent conductivities (Λ) of [N-(2-ChloroBenzylidene)-4-picolylamine] as a function of √Conc. at a temperature of (293° to 313°K) in water.

Table (3): Molar concentration, and Equivalent conductance of [N-(2-ChloroBenzylidene)-4-picolylamine] at (298K) in (methanol-water) mixture.

Conc. (Mol/lit.) $*10^{-6}$	√Conc. (Mol/lit.) $*10^{-3}$	Λ (Ω^{-1}. equive^{-1}.cm^2) at 10%	Λ (Ω^{-1}. equive^{-1}.cm^2) at 20%	Λ (Ω^{-1}. equive^{-1}.cm^2) at 30%	Λ (Ω^{-1}. equive^{-1}.cm^2) at 40%	Λ (Ω^{-1}. equive^{-1}.cm^2) at 50%
0.5187	0.7202	481.9177	495.3725	419.2397	378.6713	330.2541
1.0043	1.0021	273.7999	263.7901	224.5274	203.7119	167.8105
1.4750	1.2145	203.3800	190.3373	170.1554	144.0660	118.6329
1.9412	1.3932	167.4152	154.2980	132.9280	114.9328	95.1122
2.4141	1.5537	144.9815	134.0488	114.4334	95.5951	79.1516
2.9116	1.7063	128.7925	119.9340	100.8537	83.7504	67.6990
3.3963	1.8429	117.7744	108.9075	92.0235	75.2657	60.8479
3.8416	1.9599	110.6311	101.1464	84.7058	68.4515	55.3070
4.2953	2.0725	104.7653	94.3646	78.9556	64.5468	51.2341
4.9081	2.2154	95.7585	88.8114	75.1139	60.0132	47.7969
5.3883	2.3212	90.9367	83.4242	70.4030	56.4796	44.0958
5.8609	2.4209	87.0167	80.8614	67.2688	53.7096	41.9502
6.2787	2.5057	83.6154	77.9453	65.0833	51.1603	39.6058
6.7379	2.5957	80.8856	74.9381	63.0235	49.5914	38.1353
7.1648	2.6767	78.1596	72.6219	61.1708	49.2146	36.5867
7.7042	2.7756	74.6340	70.0595	61.1708	47.7220	35.4904

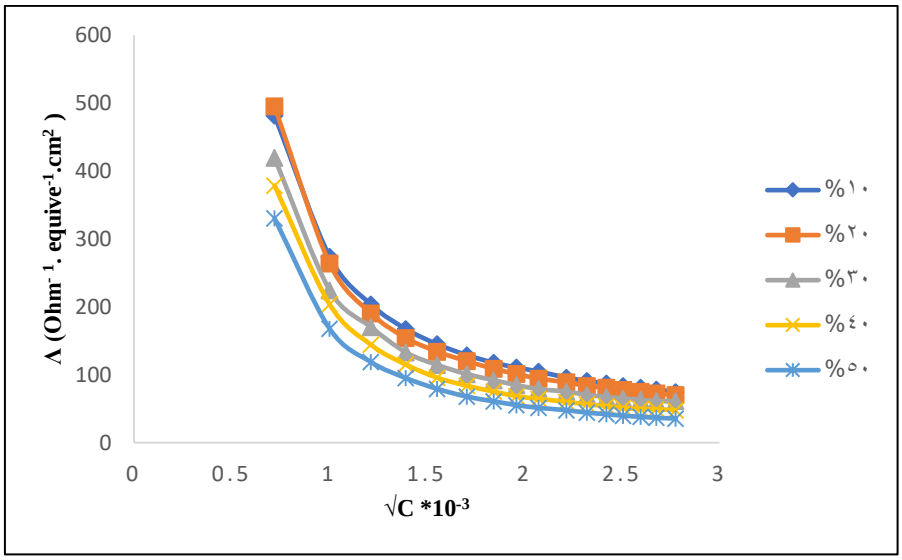


Figure 3. Equivalent conductivities (Λ) of [N-(2-ChloroBenzylidene)-4-picolylamine] as a function of √Conc. at a temperature of (298K) in (methanol-water).

When using different solvents and at different temperatures, it was found that the conductivity values increase with increasing temperature. This indicates that with increasing temperature, the ions gain more energy, which increases their ability to transmit electricity and increases their conductivity. In addition, the dielectric constant of the solvent also affects the conductivity value. Whenever the number of free ions increases, the conductivity increases. The LW equation was applied to calculate the equivalent conductivity (Λ), the association constant (Ka) and the distance between R (A°) and σΛ for the above solutions. After obtaining information about the measurements, such as: B. Fixed cell concentration (0.5 cm), concentration, equivalent conductivity values and

(density, solution viscosity and dielectric constant) changes depending on temperature and solvent, were analyzed using special programs. Tables (4, 5, & 6) give the values of Ka, Λ, R and σΛ [14].

Table (4): The values of (K_A), (Λ_o), (R) and (δΛ) for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in methanol at (293°-313°K)

T(K)	K_A	Λ_o	R (Å)	δΛ
293	4038431	153.194	1.3	0.0284
298	4968345	228.591	1.8	0.0483
303	5869144	296.308	1.9	0.0219
308	6031102	339.675	1.4	0.0422
313	6588348	449.801	1.8	0.0549

Table (5): The values of (K_A), (Λ_o), (R) and (δΛ) for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in water at (293°-313°K)

T(K)	K_A	Λ_o	R (Å)	δΛ
293	288702	64.599	1	0.0358
298	417057	75.4097	1	0.0385
303	633057	139.593	1	0.0607
308	734393	180.343	1	0.0763
313	1104288	282.654	1	0.1017

Table (6): The values of (K_A), (Λ_o), (R) and (δΛ) for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in a mixture at (298°K)

%	K_A	Λ_o	R (Å)	δΛ
10%	7439637	1163.539	1	0.7878
20%	1371383	2135.475	1	0.8244
30%	10824329	1348.244	1	0.7353
40%	7977257	709.8561	1	0.7133
50%	6633673	333.3907	1	0.8406

The results of this study indicate that when the distance between the anion is smaller than 2(Å), a cation and anion combine to form a Contact Ion-Pair (CIP). The standard deviation amount demonstrated that this equation was suitable for the investigation.

Then we calculate the thermodynamic parameters (ΔH, ΔG & ΔS) by using (Van't-Hoff) equation, by plotting the relation between $\ln K_A$ against 1/T [15].

$$LnKa = -\frac{\Delta H}{RT} + C \quad \ldots. (1)$$

$$\Delta G = -RTLnKa \quad \ldots. (2)$$

$$\Delta G = \Delta H\text{-}T\,\Delta S \quad \ldots. (3)$$

Table (7): Thermodynamic parameters for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in methanol at (293°-313°K).

T(K)	LnK_A	ΔG ($KJ.mol^{-1}$)	ΔS ($J.mol^{-1}.K^{-1}$)	ΔH ($KJ.mol^{-1}$)
293	15.2113	-37.0549	187.8149	
298	15.4185	-38.2006	188.5085	
303	15.5852	-39.2613	188.8985	17.9748
308	15.6124	-39.9789	188.1617	
313	15.7008	-40.8579	187.9642	

Figure (5): The Relation between LnK_A and 1/T for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in methanol at (293°-313°K).

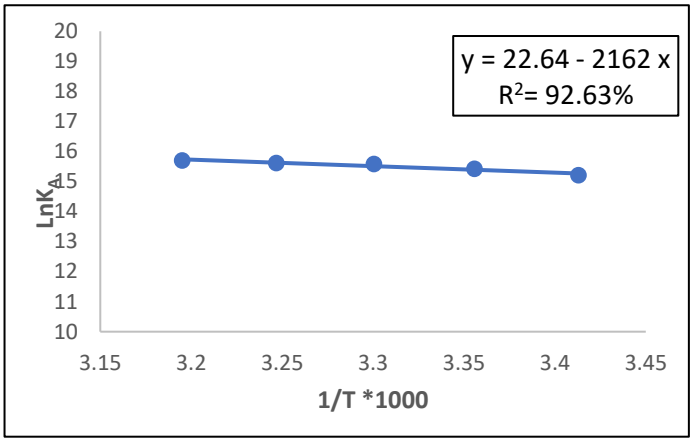
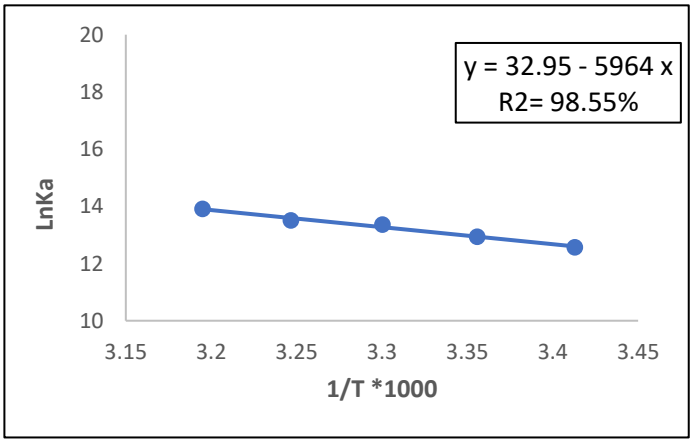


Table (8): Thermodynamic parameters for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in water at (293°-313°K).

T(K)	Ln K_A	ΔG ($KJ.mol^{-1}$)	ΔS ($J.mol^{-1}.K^{-1}$)	ΔH ($KJ.mol^{-1}$)
293	12.5731	-30.6282	273.7642	
298	12.9409	-32.0622	273.9828	
303	13.3583	-33.6514	274.7068	49.5847
308	13.5067	-34.5870	273.2848	
313	13.9147	-36.2100	274.1044	

Figure (6): The Relation between LnK_A and 1/T for (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in methanol at (293°-313°K).



The Van't Hoff equation was applied to calculate three thermodynamic values, namely ΔH ΔG ΔS, to explain the behavior of the compound in water and methanol, as shown in the tables 7&8) and Figures (5 & 6)
The enthalpy values in both solvents were positive, indicating that the reaction was endothermic, but slightly greater than in methanol in water, and the ΔG values in water and methanol were negative and close, indicating that the process was spontaneous, while the results showed that the value of ΔS was positive, increasing the randomness, i.e., H. The freedom of movement of ions in the solution is greater in water than in methanol.

Walden Product ($\eta_o\Lambda_o$):

The Walden Product can be calculated by multiplying the equivalent conductivity at infinite dilution (Λ_o) and viscosity of the solvent (η_o). The Walden Product can be used to determine the (Water-Structuring) activity [16].

Table (9): The Relation between Walden product ($\eta\Lambda$) and percentage (%) of (Methanol-Water) mixture at 298°K.

Percentage %	η_o	Λ_o (Ω^{-1}. equive^{-1}.cm^2)	$\eta_o\Lambda_o$
10	0.0013	1163.539	1.5946
20	0.0018	2135.475	3.8993
30	0.0022	1348.244	3.0760
40	0.0027	709.8561	1.9428
50	0.0031	333.3907	1.0643

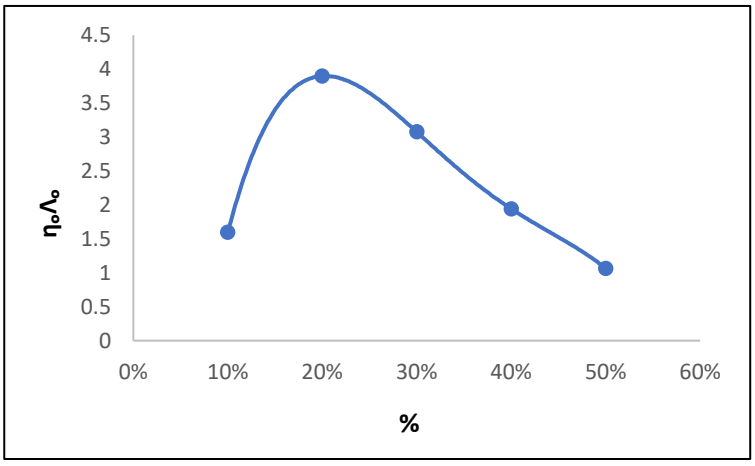


Figure (7). The Relation between Walden product ($\eta_o\Lambda_o$) and percentage (%) of (Methanol in Water) mixture at 298°K.

3.2 Theoretical Results:

The computational calculations were performed using [DFT/B3LYP/6-31G] calculation level for geometry optimization of molecular system. The following table (11) shows structural parameters calculated in different solvents (Gas, Water, and Methanol). The final geometry form of N-(2-ChloroBenzylidene)-4-picolylamine molecule in the solvents, as the COSMO model is shown below.

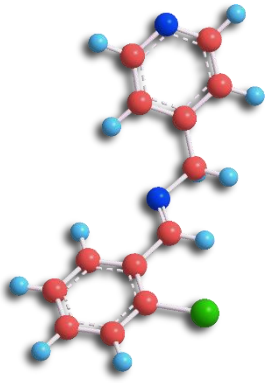
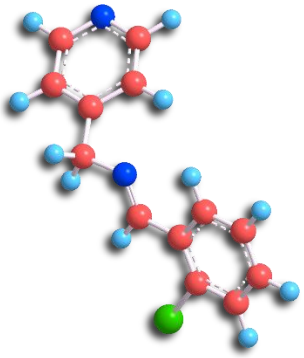
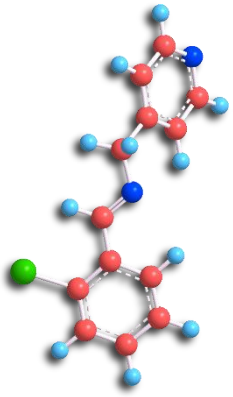
	Gas Phase	Methanol	Water
DFT/B3LYP/ 6-31G			

Table (10). (HOMO and LUMO) energies calculated at different approaches**.**

	GAS PHASE				WATER	METHANOL
	AM1	**PM3**	**HF** 6-31G	**DFT** B3LYP/6-31G	**DFT** B3LYP/6-31G	**DFT** B3LYP/6-31G
ε_{HOMO} (eV)	-0.37977	-0.36997	-0.40122	-0.26004	-0.26315	-0.26551
ε_{LUMO} (eV)	-0.00783	-0.01645	0.08638	-0.05109	-0.05995	-0.05323

Table (11). Some Descriptors for (N-(2-ChloroBenzylidene)-4-picolylamine) that calculated from (HOMO and LUMO) energies by (DFT) in different solvents.

DESCRIPTORS	**Phase**		
	Gas	**Water**	**Methanol**
ƐHOMO (eV)	-0.2687	-0.2692	-0.2670
ƐLUMO (eV)	-0.0632	-0.0634	-0.0596
GAP (Δε) (eV)	0.2055	0.2058	0.2073
Ionization potential (I)	0.2687	0.2692	0.2670
Electronic affinity (A)	0.0632	0.0634	0.0596
Hardness (Ƞ)	0.1027	0.1029	0.1036
Chemical potential (μ)	-0.1660	-0.1663	-0.1633
Electrophilicity (ω)	0.1341	0.1344	0.1286

Table (12). Global chemical reactivity indicators of (N-(2-ChloroBenzylidene)-4-picolylamine) calculated in different systems.

Descriptors	Gas	Water	Methanol
Connolly Accessible Area (A°2)	440.33	440.369	440.345
Connolly Molecular Area (A°2)	225.556	225.443	225.426
Connolly Solvent Excluded Volume (A°3)	182.076	182.588	182.563
Ovality	1.45189471312525	1.44845322866892	1.4484762252269
Principal Moment	499.973	490.631	490.557
Dipole (Debye)	3.6255	3.683	3.6833
Molecular Volume (bohr**3/mol)	2120.678	1608.721	1744.85
RMS Force (Kcal/Mol)	4.6675	4.8541	4.8522
SCF Energy (Kcal/Mol)	-669417.77	-669417.39	-669417.4
Entropy (Cal/Mol-Kelvin)	107.682	107.584	107.587
Thermodynamic Energy (Kcal/Mol)	149.176	149.099	149.101
Zero-Point Energy (Kcal/Mol)	141.964488	141.885422	141.887305
Hyper Polarizability	-93.5232	-105.923	-106.0548
Polarizability	206.9389	211.7163	211.7204

Conclusion:

In this research, the (EC) of Schiff Base Compound (N-(2-ChloroBenzylidene)-4-picolylamine) was benchmarked in different solvents including water & methanol at temperature range of (293-313K) at 5K intervals, and in (Methanol in Water) mixture at 298K in different percentage (10%, 20%, 30%, 40% and 50%). Then plotting the relation between equivalent conductivity (Λ) and square root of molar conc. ($\sqrt{}$Conc.) using Kohlrausch equation. The plotting in Figures (2, 3 and 4) shows curve lines which indicate that the compound acts as a weak electrolyte. Also, the (EC) measurements listed in Tables (1, 2 and 3) show that the (EC) of the compound increases with increasing temperature, indicating that the compound behaves as a semi-conductors.

Lee-Wheaton equation for symmetrical electrolyte (1:1) was used for the treatment of obtained data to calculate the values of equivalent conductivity at infinite dilution (Λ_o), the main distance between ions (R) and ions association constant (K_A).

The thermodynamics parameters (ΔG, ΔH, ΔS) were calculated utilizing (Van't-Hoff) equation by plotting the logarithms of the association constant (LnK_A) versus the reciprocal of temperature (1/T). The obtained positive values of enthalpy (ΔH) reveal the endothermic decomposition nature of the compound. And the values of (ΔG) are negative, which means that the ion association is spontaneous. (ΔS) values were positive which indicated to increase the entropy which refers to an increase in the mobility of ions in solvents.

Computational study performed using DFT calculation of the compound in the gas phase and methanol and water, the chemical molecule is impacted by the solvent, as seen by the variation in the three Connolly coefficient values and the size of the molecule for the gas phase. Accordingly, the analogous conductivity value decreases with increasing solvent molecule size, making it more difficult for molecules to move about in the solution. This link is also evident in the realistically computed entropy values.

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Competing Interests

The authors declare that there are no competing interests.

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