

Conductometric and Computational Study of Chloramphenicol at Different Solvents and Temperatures

Amel G. Abed  

Department of Chemistry, College of Science, University of Mosul, Mosul, Iraq.

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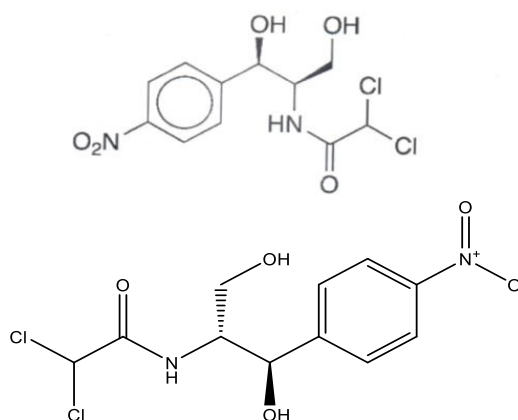
Abstract

In the present work, the electrical conductivity of chloramphenicol was measured in water and methanol at different temperature degrees 293-313 K. The parameters of conductivity equivalent conductance at infinite dilution (Λ_0), the association constant (K_A) and distance parameter (R) were all recorded by using Lee-Wheaton equation and the thermodynamic parameters (ΔH , ΔG , and ΔS) were calculated as well. The behavior of a compound can be predicted through computational calculations; taking 2,2-dichloro-N-[(1R,2S)-1,3-dihydroxy-1-(4-nitrophenyl) propan-2-yl] acetamide, for example. There is an abundance of theoretical information available about how this compound behaves in different solvents, such as water and methanol. The secret lies in analyzing the compound's HOMO and LUMO energies, which can be determined through advanced computational calculations using methods like AM1, PM3, and HF. The potential of the compound was different when changing the solvent and this is due to the value of energy and other theoretical factors like the molecular volume and Connolly parameters.

Keywords: Austin Model, Chloramphenicol, Electrical Conductivity, Hartree-Fock, Parametric Method.

Introduction

Chloramphenicol (CAP) $C_{11}H_{12}Cl_2N_2O_5$, Scheme 1 is an antibacterial agent with abroad spectrum of activity against gram-positive bacteria, gram-negative bacteria^{1,2}. So it is a medication used in the cases of infections where chloramphenicol ointments are used for treating the surgical wound infections in the plastic surgery and eye surgery^{3,4}, chloramphenicol has also been used for treating of typhoid⁵ and cholera⁶. Chloramphenicol is classified as antimicrobials that inhibits protein synthesis, and it is organo chlorine compound that is dichlorosubstituted acetamide containing a nitro benzene ring, an amide bond, and two alcohol functions and it is a white to pale yellow powder⁷.



Scheme 1. 2D Molecular structure of CAP, $C_{11}H_{12}Cl_2N_2O_5$

Because of the big importance of the antibiotics compounds, many researches about them have been carried out, e.g: a study of spectroscopic characterization of chloramphenicol and tetracycline using FT-IR and UV-Vis spectroscopy⁸ and a theoretical study of ciprofloxacin antibioticus using theory of (DFT) time – dependent density functional theory (TD-DFT), and molecular dynamics (MD) simulations⁹. In the scientific studies, it is necessary to know the behavior of electrolytes in solution so the electrical conductivity studies , one of the most important ways to show the ion-ion and the ion-solvent interaction is by noting the properties for conductivity with ions movement¹⁰. Furthermore, the effect of temperature on the conductivity measurements for the electrolyte solution with different temperature can give more information about the kind of interaction¹¹. The electrical conductivity measurements is very important and common subject for instance study of some amino acids and their complexes with some metals in different solvents and different temperatures where the values of (K_a) , (Λ_0) and (R) were calculated and thermodynamic parameters (ΔH , ΔG and ΔS) for complexes were determine¹².

In this work, the study of electrical conductivity of chloramphenicol in water and methanol were recorded at temperatures range 20-40C⁰. To uncover the secrets of the association process, the study explored the depths of each temperature using the LW equation of symmetrical electrolytes. By analyzing the results through calculating the values of enthalpy, entropy, and Gibbs free energy. Beside

Materials and Methods

The chemicals are pure powder of chloramphenicol from the state company for drugs industry and medical appliances (SDI) Samarra /Iraq, methanol from Fluka Switzerland (99.8%), water of conductivity prepared by adding a small amount of potassium permanganate and few pellets of (KOH) to the water that will be redistilled three times ¹⁵. This water used as the solvent with the specific conductivity less than (1.5×10^{-6} S/cm). A quantity of (10-3M) of the chloramphenicol solution was prepared by dissolving the necessary weight of the chloramphenicol in the water allocated for conductivity measurements. Then, the solution completely was filled with water until the pointer indicated the correct volume. This ensured that the

that the present study has been supported by the calculations of the quantum chemistry methods to study chloramphenicol solution theoretically through:

The computational chemistry proved to be a valuable apparatus to study the materials that are either impossible to be obtained or which are extremely costly. Also it assists chemists in conducting forecasts before conducting real experiments as this allows them to make better observations. The basis of most of the computational chemistry theory and computer applications is the quantum and the classical mechanics in addition to the thermodynamics and mathematical physics. The computational chemistry uses geometry to model the atoms and molecules accordingly. The most important computational techniques involve ab-initio, semi-empirical and molecular mechanics^{13, 14}. This study aims at identifying the chemical action of the chloramphenicol through the interpretations the compound-compound and the compound-solvent interactions. Moreover, there is more potential to understand the nature of ion associations in various solvents via the thermodynamic study that involved values of Gibbs free energy, entropy and enthalpy. Finally, the chloramphenicol solutions were evaluated theoretically using the quantum chemistry calculations. These calculation resulted in compatibility with the values obtained practically. So, using the three studies (the electrical, thermodynamic and the theoretical studies) was successful and characterized with agreements in terms of the results.

prepared solution was perfectly balanced and ready for use. This process was repeated for another solvent - methanol - to ensure that a comprehensive understanding of the solution's properties ensued.

Apparatus:

To measure conductivity with the powerful and computerized WTW InoLab 740 conductivity meter; equipped with platinized platinum electrodes, this meter boasts unbeatable accuracy and precision. The cell constant of 0.05582cm^{-1} and a water bath (HAKK-NK22) that maintains temperature within $\pm 0.15 \text{C}^0$, you can be sure your readings are always spot-on. Regarding the preparation of stock solutions, we rely on our

expertly calibrated instruments, which are always freshly prepared and weighed to perfection.

To measure conductivity, a precise protocol was used; started by placing a specific amount of solvent into a clean and dry conductivity cell. After weighing the cell, it was placed in a thermostated water bath at the right temperature, then a plastic syringe was used to add the stock solution to the solvent in the cell. To ensure accuracy, the syringe was weighed before and after filling it with the stock solution. After each addition, the solution was stirred with a magnetic stirrer and recorded its conductivity. This process was repeated until required stock solution had added. Finally, the cell reweighed to calculate the change in weight, which was found to be less than 0.02%. By following this rigorous procedure, precise and reliable conductivity measurements were obtained.

Computational Detail:

After verifying that the structures were drawn correctly in Chem. Draw.2D, version 16, the compound was translated to Chem. 3D and a number of theoretical calculations were carried out. Molecular dynamics and molecular mechanics (MM2) were used to minimize the problem until the molecule achieved its lowest energy state¹⁶.

To find the lowest energy level of each molecule, the minimization procedure was repeated using quantum mechanics, the Austin Model 1 (AM1) system, and then Parametric Method 3 (PM3), a

Results and Discussion

This study includes the application of Lee-Wheaton equation for the symmetrical electrolytes solution of type (1:1) of chloramphenicol in two solvents (water and methanol) at different temperature (293-313K), in this case the single symmetrical electrolyte solution of the Eq. 1 has the form:

$$\Lambda_{\text{equiv}} = f(\Lambda_0, R, K_A) \dots \dots \dots 1$$

where

Λ_0 = limiting equivalent conductance

K_A = association constant

R = distance parameter

semi-empirical method for quantum molecular electronic structure computations.

The Gaussian Interface version 09 software was used to determine various attributes and parameters for each molecule after knowing the global state as described in Fig. 1.

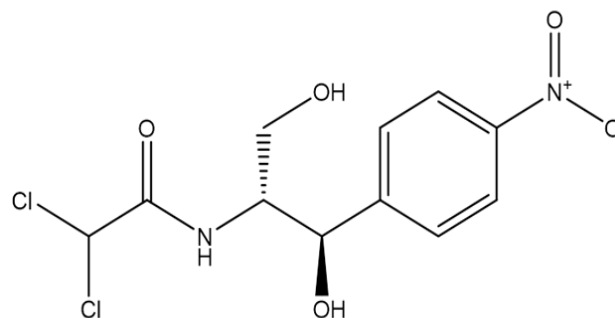
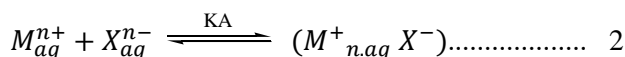


Figure 1. 2D chemical structure of 2,2-dichloro-N-[(1R,2S)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl] acetamide

In addition to RHF (restricted Hartree-Fock: closed shell), the wave function was used for optimization up to the root mean square (RMS) gradient reaching a value less than 0.01 kcal/mol. After completing the minimization energy of the molecule, the description in the water and methanol must be calculated initially using the PM3 method, and then using the 6-311G(d) base established by HF. The best conformer with the least energy was therefore taken into account as the actual sample representing the molecule for measurement, and this sample was utilized as a starting model for other calculations¹⁷.

Lee and Wheaton^{18, 19} give the Eq 2 for a symmetrical electrolyte of type (1:1) as:



where (M^{n+}) is the positive ion and (X^-) is the negative ion.

K_A is the association constant.

The values of molar concentration (Conc.) and equivalent conductance for the solution of chloramphenicol in water at different temperature are shown in Table 1.

Table 1. Molar concentration (Conc.) and equivalent conductance of chloramphenicol in water at different temp.

Conc. $\times 10^{-5}$ mole /litter	Λ $\text{ohm}^{-1}.\text{equi}^{-1}$ $\cdot\text{cm}^2$ 293K	Λ $\text{ohm}^{-1}.\text{equi}^{-1}$ $\cdot\text{cm}^2$ 298K	Λ $\text{ohm}^{-1}.\text{equi}^{-1}$ $\cdot\text{cm}^2$ 303K	Λ $\text{ohm}^{-1}.\text{equi}^{-1}$ $\cdot\text{cm}^2$ 308K	Λ $\text{ohm}^{-1}.\text{equi}^{-1}$ $\cdot\text{cm}^2$ 313K
0.69067	7.23928	14.83324	25.29212	35.24160	53.30420
1.29383	5.79671	11.02863	19.32819	30.91390	33.18040
1.80221	5.54871	10.19798	18.21174	19.2825	26.67196
2.48403	5.03213	10.98392	16.71430	16.03704	22.04864
2.96014	5.06730	10.37064	18.01483	14.47807	21.07900
4.66793	5.89125	11.36908	18.26090	12.29496	20.04967
5.00029	5.99964	11.56599	18.41023	10.16276	18.25980
5.49209	5.91759	12.03959	17.84131	9.47175	17.03825
6.01448	5.40361	11.17805	17.47759	9.344123	16.42776
6.47756	5.01731	10.36375	16.08601	9.39000	15.44321
6.89566	4.71310	9.57055	14.95240	9.23782	14.74573
7.25639	4.47880	9.08114	14.19414	9.19791	14.43208

The plots of the values of equivalent conductance (Λ_{equiv}) against the square root of the molar concentration of the chloramphenicol solution in water are shown below in Fig. 2.

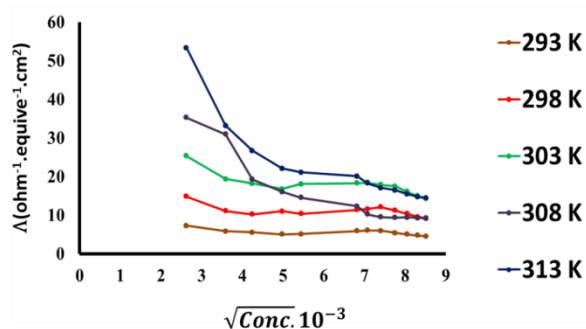


Figure 2. The relation between the square root of concentration and the equivalent conductance of chloramphenicol in water at different temperature

It can be seen from Table 1 and Fig. 2 the increase in the values of equivalent conductance with increasing the temperature and the solution behavior as weak electrolyte. Because of the big difference of dielectric constant between water and methanol, it was studied in methanol at the same different temperature, Table 2 shows the values of concentration with the values of equivalent conductance (Λ_{equiv}) for the solution of chloramphenicol in methanol as described in Fig. 3.

Table 2. Molar concentration (Conc.) and equivalent conductance of chloramphenicol in methanol at different temperature

Conc. × 10 ⁻⁵ mole /litter	Λ ohm ⁻¹ .equive ⁻¹ .cm ² 293K	Λ ohm ⁻¹ .equive ⁻¹ .cm ² 298K	Λ ohm ⁻¹ .equive ⁻¹ .cm ² 303K	Λ ohm ⁻¹ .equive ⁻¹ .cm ² 308K	Λ ohm ⁻¹ .equive ⁻¹ .cm ² 313K
3.82508	2.03241	1.15012	1.25032	1.30013	1.18133
6.29328	1.81320	1.09014	1.08002	1.16122	1.05355
8.52818	1.75887	1.02011	1.03142	1.11102	0.99243
11.47967	1.74221	0.96566	0.98790	1.05021	0.97445
13.83230	1.80736	0.97102	0.97863	0.99800	0.94761
16.06254	1.86769	0.98334	0.99260	0.99684	0.96834
18.47570	1.89438	1.02223	1.04409	0.99423	0.95882
20.72553	1.92998	1.04361	0.94591	1.00760	0.96985
23.23585	1.93666	1.08432	0.86770	1.02338	0.99288
27.93659	1.92185	0.97808	0.79269	0.96162	0.98737
29.91898	1.73171	0.89435	0.73849	0.91339	0.90481
34.64767	1.71122	0.83377	0.96294	0.87454	0.78856

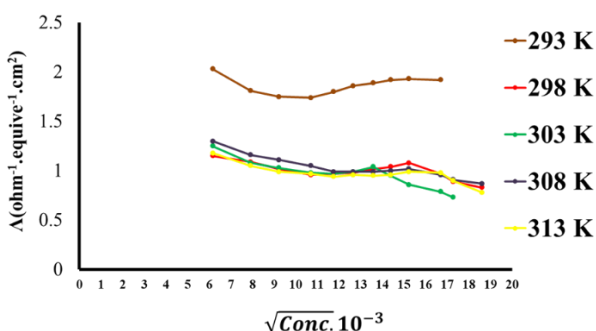


Figure 3. The relation between the square root of concentration and the equivalent conductance of chloramphenicol in methanol at different five temperatures

From the results above for methanol solution, it can be seen that the values of equivalent conductance of the solution increase with increasing temperature at the level $\Lambda_{298k} > \Lambda_{303k} > \Lambda_{308k}$. This is due to the association between ions happening with increasing temperature.

At 293k and due to the large size of molecules there is an increase in the degree of freedom for the molecules of chormaphenicol upon the association between methanol and CAP leading to a height in the equivalent conductance more than the other states of temperatures (the equivalent conductance value is not just determined by one factor, but by a combination of several factors. The structure, molecular volume, and type of solvent all play an important role in influencing the transition of ions)^{20, 21} as:

$\Lambda_{293k} > \Lambda_{298, 303}$ and $308k$

The way a solution behaves can be quite fascinating. For instance, as the temperature rises, the process of association between positive and negative ions slows down. This happens because the volume of methanol molecules is larger than that of water, and this difference becomes more pronounced at higher temperatures, this intriguing behavior is especially noticeable in solutions at 313K.

Lee-Wheaton equation for the electrolyte solution of kind (1:1) has the public formula (Eq. 3):

$$\Lambda = \Lambda^\circ [1 + C_1(KR)(\epsilon K) + C_2(KR)(\epsilon K)^2 + C_3(KR)(\epsilon K)^3] -$$

$$\frac{PK}{1 + KR} \left\{ 1 + C_4(KR)(\epsilon K) + C_5(KR)(\epsilon K)^2 + KR / 12 \right\}$$

..... 3

Where

$$\epsilon = \frac{|z|^2 e^A}{DKT}$$

$$P = \frac{F\delta/z}{3\pi y}$$

$$K^2 = \frac{8\pi N^2 e/z^2 C}{1000DKT}$$



F= faraday constant = 9.04867×10^4 coulombs / eguiv

$$\delta = \text{conversion factor} = \frac{1}{299.7925}$$

= (volt – electrostatic) e.u.s=1/299.7925

C= concentration (mole/Liter)

D= Dielectric constant of solvent

η = viscosity of solvent . where the meanings for all symbols of equation (3) were available on the study of Lee-Wheaton¹⁸, the conductometric study of the complexes of amino acids ¹², and the study of conductivity of aspartic acid complexes ²².

Calculation of K_A by Computer Program

Scientists determine the association constant (K_A) and equivalent conductance (Λ_{equiv}) values for various solvents at different temperatures using the Lee-Wheaton equation and a computer program to calculate these values based on the cell constant (0.5)cm-1, density (gm/cm³), molecular weight of the compound (CAP), viscosity (η), and dielectric constant (D). The program, known as Mr2, does all the heavy lifting by analyzing the data and providing the molar concentrations and equivalent conductance values. The analysis results not only give us the K_A and Λ° values but also the distance parameter (R) and standard deviation ($\sigma\Lambda$).

According to the Lee-Wheaton equation the values of association constant (K_A) equivalent conductance (Λ_{equiv}) were calculated by computer program through giving the information about cell constant 0.5 cm⁻¹, density gm/cm³ for every solvent and at each temperature, molecular weight for compound (CAP), in addition to the values of viscosity (η) in poise and dielectric constant (D) by using computer program (Mr2) for data analysis which includes values of molar concentrations and equivalent conductance.

The analysis results presented the values of the association constant (K_A), equivalent conductance at infinite dilution (Λ°), distance parameter (R) and the standard deviation ($\sigma\Lambda$) as shown in Eq.4.

$$\sigma(\Lambda) = \sqrt{\frac{\sum_{n=1}^{NP} (\Lambda_{\text{cal}} - \Lambda_{\text{exper}})^2}{NP}} \dots\dots\dots 4$$

NP= Number of points

The calculated results of the analysis of the chloramphenicol solutions firstly in water and secondly in methanol at different temperature contains the values of limiting equivalent conductance (Λ°), association constant (K_A), the distance parameter (R) and the best fit data standard deviation $\sigma\Lambda$ (Λ), are shown in Tables 3 and 4.

Table 3. The values of (Λ°),(K_A),($\sigma\Lambda$) and (R)for the chloramphenicol solution in water at different temperature

TK	Λ° ohm ⁻¹ .equiv ⁻¹ .cm ²	K_A	$\sigma\Lambda$	R(A ^o)
293	53.108	294.273	0.0494	6
298	13.378	29.029	0.0093	2
303	21.160	971.505	0.0148	11
308	38.810	109049.820	0.0247	23
313	8.456	75767.300	0.1169	1

Table 3 presents an intriguing observation: as the temperature rises within the 298-308K range, the equivalent conductance (Λ°) and (K_A) values experience an upward trend. This can be attributed to the influence of temperature on solution properties, such as the decreasing solvent dielectric constant. Notably, (K_A) values detect a significant spike at 308K compared to 303K, suggesting an increase in ionic aggregations²³ and short-range commutability reaction ²⁴. Furthermore, at 313K, the associated ion pair decreases and the distance parameter approaches the contract ion pair (1.00 Ao), resulting in small values of ($\sigma\Lambda$) overall. These insights shed light on the dynamic relationship between temperature and solution properties, offering valuable implications for future studies.

Table 4. The values of (Λ°), (K_A), ($\sigma\Lambda$) and (R) for the chloramphenicol solution in methanol at different temperature

TK	Λ° ohm ⁻¹ .equiv ⁻¹ .cm ²	K_A	$\sigma\Lambda$	R(A ^o)
293	3.878	12.584	0.0134	10
298	2.620	24.282	0.0829	10
303	3.130	13.990	0.0458	10
308	3.021	44.212	0.0158	10
313	3.181	56.363	0.0213	10

In spite of the behavior of the solution in methanol, it can be seen from the Table 4, the possible values are ranging from 2.6 to 3.1 ohm⁻¹.equiv⁻¹.cm² for (Λ°) at the temperatures 298-303-308 and 313k and

there is sort of increase with increasing temperature which, due to the decreasing of the medium viscosity and in general the values of (K_A) increase with increasing temperature because of decrease in dielectric constant and density of the solvent with increasing temperature. (R) values indicate that the ions was separated by several molecules of methanol and the few values of (\square) were noted.

Determination the Thermodynamic Parameters (ΔH , ΔG ; ΔS):

Depending on the Van't Hoff (Eq. 4).

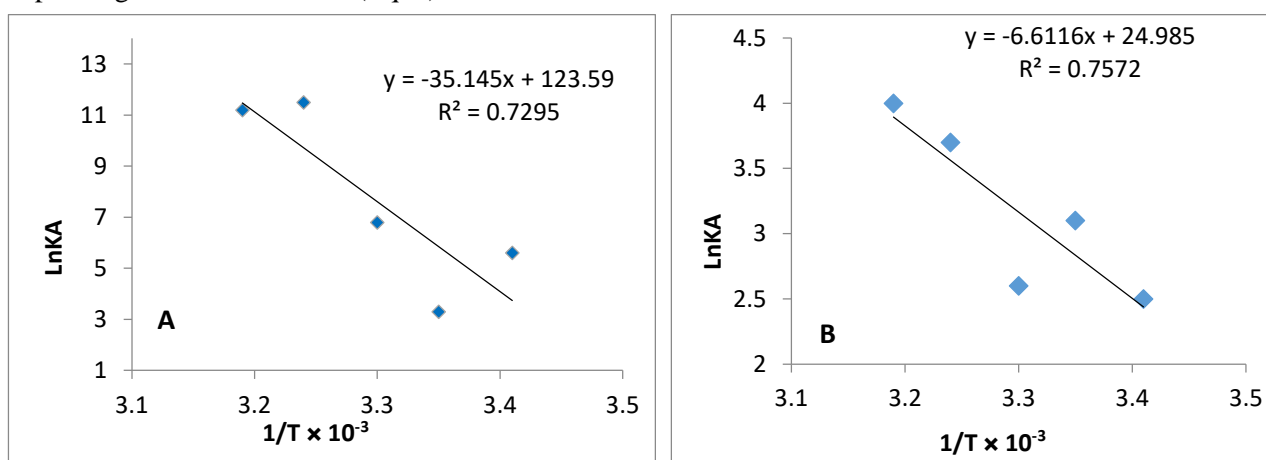


Figure 4. The relationship between the $\ln K_A$ and $1/T$ of the solution of chloramphenicol in (A) –water , (B) – methanol

From Fig. 5 the values of ΔH were calculated.

ΔG were obtained from the values of K_A and temperatures from the Gibbs free energy (Eq. 6):

$$\Delta G = -RT \ln K_A \dots\dots\dots 6$$

Also the values of (ΔS) were calculate from Eq. 7:

$$\Delta G = \Delta H - T \Delta S \dots\dots\dots 7$$

The results of the values of ΔG , ΔS , ΔH for the solution of chloramphenicol in water firstly and in methanol secondly are shown in Table 5 and 6.

Table 5. Thermodynamic parameter of chloramphenicol solution in water

TK	- ΔG kJ.mol ⁻¹	ΔS J.mol ⁻¹ .K ⁻¹	ΔH kJ.mol ⁻¹	$\ln K_A$
293	13.83	1044.436	292.19	5.68
298	8.32	1008.422		3.36
303	17.30	1021.419		6.87
308	29.67	1045.000		11.59
313	29.22	1026.869		11.23

$$\ln K_A = -\frac{\Delta H}{R} \cdot \frac{1}{T} + C \dots\dots\dots 5$$

The thermodynamic functions can be calculated by using the values of association constant (K_A) at different temperatures, by plotting the values of ($\ln K_A$) against the values of ($1/T$) for the solutions in different solvents results a relationship as shown in Fig. 4.

Table 6. Thermodynamic parameter of chloramphenicol solution in methanol

TK	- ΔG kJ.mol ⁻¹	ΔS J.mol ⁻¹ .K ⁻¹	ΔH kJ.mol ⁻¹	$\ln K_A$
293	6.16	208.6	54.96	2.53
298	7.87	210.8		3.18
303	6.62	203.2		2.63
208	9.67	209.8		3.78
313	10.48	209.1		4.03

From Table 5, it was evident that (ΔH) value of the ionic aggregations is positive for the chloramphenicol solutions (endothermic) and this because the solute molecules are surrounded by the dissolvent (water), which possesses a high dielectric constant and this eventually leads to the breaking of the bonds of the solute ions and forming more hydrogen bonding²⁵. Moreover, from Table 6 it was clear that ΔH value of the ionic aggregations is positive chloramphenicol solutions in question (endothermic) and this is because the attraction force between the solute molecule is big and as the dissolvent is characterized with low dielectric constant, then its capability of breaking the bonding

between the solute molecules is weak and so the ionization energy is bigger than the dissolution and thus ΔH value is positive²⁶. As for all results above about the thermodynamic study Gibbs free energy ΔG has negative values indicators to the spontaneous association and compatible with the relation.

$$\Delta G = -RT \ln K_A$$

ΔS positivity is due to the disorientation of the solvent separated ion pair because of the muss of the arrangement of the molecules of solvent when the ionic pair formation and the orientation of the solvent molecules become small at the formation of the ion-pair (the solution contains the ion pairs together with free molecules) as well as the positive value of ΔS and its different values for solvents due to the mathematical process resulting from the application of the laws:

$$\Delta G = \Delta H - T \Delta S$$

$\Delta H \rightarrow$ positive value

$\Delta G \rightarrow$ negative value

And that according to the negative values of slope.

Amongst the studies that had similar results to the ones in this paper: Thermodynamic parameters calculation ΔH , ΔG , ΔS for the complex $[\text{Co}(\text{C}_9\text{H}_9\text{NO}_3)_3] \text{Cl}$, which indicated the positive values of each of ΔH and ΔS and the negative values of ΔG . Also, the values of ΔS were higher in the water solvent than the values in methanol. This was all mentioned in the study entitled: "Conductometric study for the ionic association of some transition metals complexes with some amino acids in different solvents"¹².

The Result of Theoretical Study:

Table 7 reveals some fascinating insights about 2, 2-dichloro-N-[(1R, 2S)-1, 3-dihydroxy-1-(4-

nitrophenyl) propan-2-yl] acetamide. The computed descriptors are critical in understanding this compound's behavior in different solvents. It is important to note that the values of these descriptors are dependent on the solvent used, which means they can vary significantly. However, when the PM3 method was used to calculate the descriptors, a little difference was noticed in the results of the employed two solvation models. This method is a quasi-experimental approach that is perfect for comparison purposes. Interestingly, a great convergence was observed in the values obtained, with the same three values of Connolly being present across all the solvents being tested. What is even more intriguing is the effect the solvent has on the molecule's association volume, which is a clear indication of how solvent molecules gather around this compound. As observed, the molecular volume of the 2,2-dichloro-N-[(1R,2S)-1,3-dihydroxy-1-(4-nitrophenyl) propan-2-yl] acetamide varies with different solvents, which is a testament to the solvent's influence on this molecule.

The entropy which is calculated theoretically can show its value in each method used to calculate (AM1, PM3, and HF) in water more than in methanol which refers to its free mobility in water greater than methanol. These results are identical to the entropy value which results from the experiment.

These calculations depended on the HOMO and LUMO energies, which had a direct correlation to the compounds' physical attributes and stability. The compound may become more stable by lowering the HOMO's energy. To forecast its response, the HOMO is insufficient on its own. When the HOMO has little energy, the relative LUMO and HOMO occupancy, as well as the LUMO's electricity, all have a role²⁷⁻²⁹.

Table 7. Values of descriptors in water, and methanol, were calculated by (AM1, PM3, and HF)

Descriptors	AM1		PM3		HF	
	Water	Methanol	Water	Methanol	Water	Methanol
E_{HOMO} (eV)	-0.39222	-0.43332	-0.37853	-	-0.36944	-0.37011
E_{LUMO} (eV)	-0.05825	-	-0.05082	-0.05825	0.03471	0.03328
Finished Energy Kcal/Mole	-124.96	-130.88	-123.84	-131.56	-	-
Molecular Volume (MV) bohr**3/mol	2528.663	2525.847	2458.802	2456.802	1139643.7	1139643.26
Connolly Accessible Area (CAA) Å ²	475.432	475.422	465.271	465.26	461.428	461.064



Connolly Molecular Area (CMA) Å	465.154	239.738	239.833	238.037	239.833	238.51
Connolly Solvent Excluded Volume (CSEV) Å ³	200.829	200.765	199.233	199.069	198.883	199.233
Entropy Cal/Mol. Kelvin	127.433	123.935	127.943	124.098	128.177	124.803
Thermodynamic Energy (Kcal/Mol)	170.452	170.444	170.422	170.410	170.377	170.358

Conclusion

The study shows the effect of solvent on the ionic behavior for (CAP), through the recorded results of conductivity measurement of dilute concentrations of (CAP) in water and methanol at different five temperatures 20-40C⁰. And this results were analyzed in accordance to the Lee-Wheaton equation for dilute solutions by finding the conductivity values. The association constant (Ka) and the distance parameter (R) are affected by the difference in the values of dielectric constant and viscosity of each solvent, it can be inferred from the

results of thermodynamic part that the association process is endothermic (+ΔH) and the increasing of degrees of freedom(+ΔS) by using computational theory (AM1, PM3 and HF).

The main interest is to find an accurate and effective solution model for quasi-experimental quantum mechanics and HF methods applied to 2,2-dichloro-N-[(1R,2S)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl] acetamide in the context of a computer-aided conduction study.

Acknowledgment

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Authors' Declaration

- Conflicts of Interest: None.
- I hereby confirm that all the Figures and Tables in the manuscript are mine. Furthermore, any Figures and images, that are not mine, have been

- included with the necessary permission for re-publication, which is attached to the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at University of Mosul.

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دراسة توصيلية وحسابية للكلورامفينيكول في مذيبات ودرجات حرارية مختلفة

امل غازي عبد

قسم الكيمياء، كلية العلوم، جامعة الموصل، الموصل، العراق.

الخلاصة

في العمل الحالي ، تم قياس التوصيلية الكهربائية للكلورامفينيكول في الماء والميثانول عند درجات حرارة مختلفة 293-313 كلفن . تم تسجيل كل من المواصلة المكافئة عند درجة التخفيف اللانهائي (Λ_0) وثابت التجمع الايوني (K_A) والمسافة بين الايونات (R) باستخدام معادلة لي ويتون وتم حساب المعلمات الديناميكية الحرارية (متغير المحتوى الحراري، طاقة جيبس الحرة، متغير العشوائية) وبالمثل ، هناك معلومات نظرية وفيرة حول سلوك المركب مع المذيبات المختلفة (الماء والميثانول) من خلال حساب طاقات أعلى مدار جزيئي مشغول وادنى مدار جزيئي مشغول من المركب 2،2-ثنائي كلورو -N - [1R,2S]-1،3-ثنائي هيدروكسي-1- (4- نيتروفينيل) بروبان-2-يل [أسيتاميد عن طريق الحسابات الكومبيوترية (AM1, PM3, HF) وكانت إمكانات المركب مختلفة عند تغيير المذيب نتيجة لتباين قيمة الطاقة والعوامل النظرية الأخرى مثل الحجم الجزيئي ، معلمات كونولي.

الكلمات المفتاحية: نموذج أوستن، كلورامفينيكول، التوصيلية الكهربائية، هار تري فوك، البارامترية.