

DETERMINING THE ACTIVITY COEFFICIENT AND IONIC ATMOSPHERE THICKNESS USING ELECTROCHEMICAL METHODS TO ASSESS THE IMPACT OF SALTS ON GALLICONE

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Abstract:

In this research, the relationship between electrical conductivity (Λ) for strong electrolytes and ionic strength was explored using monovalent and trivalent strong electrolytes, such as Potassium Chloride (KCl) and Chromium(III) Chloride (CrCl_3), in various ratios ranging from 0.1:0.2 to 0.1:0.6. The impact of these electrolytes on unsaturated aromatic compounds (gallicones), prepared from the reaction of 4-aminoacetophenone with 4-nitrobenzene, was observed, and their electrical conductivity was measured. It was inferred that conductivity increases incrementally with the use of KCl, whereas with CrCl_3 , the increase was consistent. From the measurements, ionic strength was calculated based on the relationship between ionic strength and electrical conductivity ($\Lambda \cdot I = F$). Additionally, the activity coefficient was determined along with the thickness of the ionic atmosphere for the reaction. This relationship allows for the direct calculation of ionic strength by measuring the conductivity of any unknown sample and provides more accurate, straightforward, and less complex results. Furthermore, the order of the reaction was calculated and found to be second-order, from which the reaction rate constant was computed at each concentration. ZAZB was calculated using the Bronsted-Bjerrum relationship, indicating a negative value which suggests that the reaction progresses with an increase in the negative direction.

Keywords: Electrolytes, Electrical Conductivity, Ionic Strength, Gallicones, Reaction Kinetics

Introduction:

Various theories on the conductivity of electrolytes have been extensively reviewed by numerous researchers. The modern theory of electrolyte conductivity was developed by Debye-Hückel and later refined by Onsager through studies on the behavior of ions in electrolytic solutions. It has been deduced that due to the electrical attraction between positive and negative ions in an electrolytic solution, ions cluster around a central ion as if located at the center of a sphere surrounded from all sides at varying distances. The ion at the center of this sphere is known as the central ion, and the ions and solvent molecules within the surrounding shell form what is known as the ionic atmosphere. The net charge within the ionic atmosphere is equal in magnitude but opposite in sign to that of the central ion. Under normal conditions, without an applied electric field, this ionic atmosphere remains uniformly spherical.

The activity coefficient of an ion decreases with increasing ionic strength of the solution, with a more significant decrease observed for ions carrying multiple charges. This rule applies to dilute solutions, but as the concentration of the electrolytic solution exceeds 0.1M, where the radius of the ionic atmosphere becomes comparable to that of the central ion, Debye-Hückel introduced modifications to the equation. The sum of electrostatic interactions between ions plays a crucial role in determining the thermodynamic conductivities of strong electrolyte solutions, which is termed the activity coefficient.

All solutions contain ions and charged particles that deviate from ideal behavior, and the degree of deviation is proportional to the electrical charge resulting from the ions and charged particles.

The activity coefficient of an electrolyte clearly depends on the concentration. In dilute solutions, the intermolecular forces are simple Coulombic attractions and repulsions, where the ions are sufficiently spaced apart to prevent any significant attraction between them, and the activity coefficient approaches one. This effect is more pronounced for ions with higher charges and solvents with low electrochemical constants, where the electrostatic environmental effects are stronger. A study was conducted to explore the relationship between conductivity and ionic strength for electrolyte solutions (KCl, CrCl₃) with different ratios ranging from 0.1:0.2 to 0.1:0.6.

Research Objective:

- To monitor the reaction process between monovalent and trivalent salts and their effect on unsaturated compounds (gallicones) using an electrochemical method.
- To determine the reaction order and calculate the reaction rate constant.
- To calculate the ionic strength (I) and the activity coefficient (F) for the reaction.
- To compute the thickness of the ionic atmosphere (d).

Literature Review:

In 2009, researcher Iqbal Salman studied the relationship between the electrical conductivity of strong electrolytes and ionic strength using divalent strong electrolytes (sodium carbonate, sodium sulfate) at concentrations ranging from 0.01M to 0.1M. The activity coefficient (F) was also calculated, showcasing a method that directly calculates ionic strength by measuring the conductivity of any unknown sample, providing more accurate results simply and with less effort.

In the same year, Amer Dawood studied the relationship between electrical conductivity (Cond) and ionic strength (I) in aqueous solutions of the following electrolytes: (NaCl, NaCO₃, NaNO₃, Na₂SO₄, K₂SO₄, CuSO₄, MgSO₄.7H₂O) at concentrations ranging from 0.1 to 1 molar at 25 degrees Celsius. Ionic strength was calculated from electrical conductivity measurements, showing that conductivity increases with ionic strength in the following order: K₂SO₄ > MgSO₄ > CuSO₄ > Na₂SO₄ > Na₂CO₃ > NaCl > NaNO₃

A mathematical relationship was also developed in this research to calculate the thickness of the ionic atmosphere (d) from the electrical conductivity measurements of electrolyte solutions:
$$d = 4.3 \times [2(F \cdot \text{Cond})]^{-1/2}$$

Electrolyte Solutions:

Electrolyte solutions are those substances whose solutions have the ability to conduct electric current. Examples include solutions of acids, bases, and salts. The ability of electrolytes to conduct electricity is due to their dissociation into ions in solution, where these ions are capable of moving and transferring electricity throughout the solution. Electrolytes are divided into two types: weak electrolytes and strong electrolytes.



Weak Electrolytes are those substances that partially dissociate into their ions in solution, resulting in weak electrical conductivity due to the low number of ions produced from their dissociation. Examples include carbonic acid (H₂CO₃) and acetic acid (CH₃COOH).

Strong Electrolytes are substances that almost completely dissociate into ions in their solutions, resulting in very high electrical conductivity. This category includes strong acids, strong bases, and their salts. Strong acids completely dissociate to produce a very large number of hydrogen ions, such as:

1. **Potassium Chloride (KCl)** is a chemical compound with the formula KCl. It is odorless in its pure state. Its crystals are white or colorless and glassy. Its crystal structure easily cleaves in three directions. Potassium chloride dissolves well in water, approximately 34g per 100 ml of water at 20°C. In contrast, potassium chloride is practically insoluble in most organic solvents. Its molecular weight is 74.551 g/mol and its melting point is 790°C.
2. **Chromium(III) Chloride (CrCl₃)** is a chemical compound in the form of a crystalline powder that is violet (anhydrous) or dark green. The oxidation state of chromium in this compound is +3. The anhydrous form of chromium chloride has low solubility in water, but in the presence of traces of chromium(II), a rapid and exothermic dissolution process occurs and the green hydrate form of chromium(III) chloride forms, involving six water molecules linked to the central chromium atom in its crystal structure.

The **Bronsted-Hjerrum hypothesis** includes the effect of salt addition on the rate of reaction. According to this hypothesis, reactions between ions proceed through the formation of complex intermediate compounds (Intermediate Complex), which then dissociate into the reaction products. The reaction between ions A and B, which have charge factors ZA and ZB respectively, can be represented by the following equation:



Bronsted and Hjerrum also found a secondary relationship based on the Debye-Huckel equation:

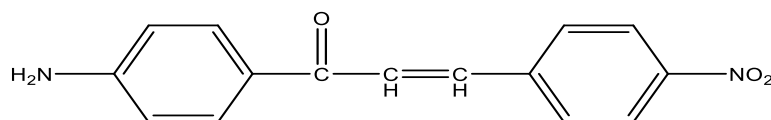
$$\log K = \log K^{\circ} + A\Delta Z^2 \sqrt{\mu}, \quad pK = pK^{\circ} - AZ^2 \sqrt{\mu}$$

Here, K is the reaction rate constant, C is a constant concentration, and μ is the ionic strength within the reaction environment. This mathematical relationship illustrates that adding a neutral salt to a specific reaction accelerates the reaction between ions carrying similar charges. The product of ZAZB will have a positive value and slows the reaction if the ions carry different charges and does not affect the reaction rate if one of the reactant ions is uncharged.

Chalcones: Chalcones are α , β -unsaturated carbonyl compounds, with chalcone itself being (1,3-diphenyl-2-propen-1-one). Other names for it include benzalacetone or phenyl styryl ketone. It is a ketonic compound containing two benzene rings connected by a carbonyl group linked with a double bond at the α , β position. In addition to the term chalcone, these compounds contain substituted groups on the benzene ring in various positions (o, m, p). The presence of two aromatic rings at the ends of the chalcone shows the planarity of the rings with the (C=C-C=O) system, which reduces the effect of substituent groups, whether they are electron-withdrawing or electron-donating.

The name chalcone was first used by researchers Tambor and Kostaneck for the purpose of preparing colored compounds. Both researchers managed to prepare yellow crystalline compounds that are insoluble in water but soluble in organic solvents. Chalcones are important for their varied uses as a material of special importance in many reactions that produce

important medical and industrial products, and the structure below illustrates the chalcone used in this study.



Chemical Formula: $C_{15}H_{12}N_2O_3$

Molecular Weight: 268.27

Elemental Analysis: C, 67.16; H, 4.51; N, 10.44; O, 17.89

M.P : 207 C°

Practical Section:

Prepared Standard Solutions:

- Chalcone Solution (0.001M):** Prepared by dissolving 0.0127g of yellow chalcone powder in a quantity of high-purity ethanol (99.9%), then diluting to the mark in a 50 ml volumetric flask.
- Potassium Chloride (KCl) Solution (0.001M):** Prepared by dissolving 0.0037g of crystalline KCl powder in a quantity of high-purity ethanol (99.9%). The solution was heated slightly to aid the dissolution of KCl in the organic solvent, as KCl is poorly soluble in organic solvents. The volume was then adjusted to the mark in a 50 ml volumetric flask.
- Chromium(III) Chloride (CrCl₃) Solution:** Prepared by dissolving 0.008g of green crystalline CrCl₃ powder in a quantity of high-purity ethanol (99.9%) and diluting to the mark in a 50 ml volumetric flask.

Methodology:

First: Measurement of Conductivity and Calculation of Ionic Strength, Activity Coefficient, and Ionic Atmosphere Thickness for KCl:

- A mixture of 0.1 ml of chalcone with various volumes of KCl (0.6, 0.5, 0.4, 0.3, 0.2 ml) was prepared. Conductivity was measured over a period, and ionic strength, activity coefficient, and ionic atmosphere thickness were calculated using the following equations:
 - $I = \frac{1}{2} \sum c_i Z_i^2 = \frac{1}{2} \sum c_i Z_i^2$
 - $I = F \cdot A_i = F \cdot \text{cond} \cdot A_i = F \cdot A$
 - $d = 4.3 \times [2(F \cdot \text{Cond})]^{-1/2} = 4.3 \times \left[2(F \cdot \text{Cond}) \right]^{-1/2}$

The results are shown in the tables and figures below:

Table 3: Conductivity Values for KCl-Chalcone Mixture (2:1 Ratio)

Ionic Atmosphere Thickness $d(A_o)d(A^o)d(A_o)$	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda(\mu S)$	Conductivity (μS)
6.799	2.778	0.2	7200	7200
6.799	2.614	0.2	7650	7650

6.799	2.532	0.2	7900	7900
6.799	2.525	0.2	7922	7922
6.799	2.469	0.2	8100	8100
6.799	2.454	0.2	8150	8150
6.799	2.424	0.2	8250	8250
6.799	2.367	0.2	8450	8450
6.799	2.299	0.2	8700	8700
6.799	2.281	0.2	8770	8770

Table 4: Conductivity Values for KCl-Chalcone Mixture (3:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere $d(A^o)d(A_o)d(A_o)$	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda(\mu S)$	Conductivity (μS)
5.551		4.792	0.3	6260	6260
5.551		4.129	0.3	7266	7266
5.551		3.879	0.3	7733	7733
5.551		3.689	0.3	8133	8133
5.551		3.629	0.3	8266	8266
5.551		3.521	0.3	8521	8521
5.551		3.409	0.3	8800	8800
5.551		3.403	0.3	8816	8816
5.551		3.238	0.3	9266	9266
5.551		3.183	0.3	9426	9426

Table 5: Conductivity Values for KCl-Chalcone Mixture (4:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere $d(A^o)d(A_o)d(A_o)$	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda(\mu S)$	Conductivity (μS)
4.807		8.556	0.4	4675	4675
4.807		7.111	0.4	5625	5625
4.807		7.097	0.4	5636	5636
4.807		7.048	0.4	5675	5675
4.807		6.957	0.4	5750	5750
4.807		6.867	0.4	5825	5825
4.807		6.695	0.4	5975	5975
4.807		6.691	0.4	5978	5978
4.807		6.679	0.4	5989	5989
4.807		6.668	0.4	5999	5999

Table 6: Conductivity Values for KCl-Chalcone Mixture (5:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere $d(A_o)d(A^o)d(A_o)$	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
4.3		13.441	0.5	3720	3720
4.3		12.69	0.5	3940	3940
4.3		12.563	0.5	3980	3980
4.3		12.438	0.5	4020	4020
4.3		12.376	0.5	4040	4040
4.3		12.315	0.5	4060	4060
4.3		11.874	0.5	4211	4211
4.3		10.994	0.5	4548	4548
4.3		10.922	0.5	4578	4578
4.3		10.841	0.5	4612	4612

Table 7: Conductivity Values for KCl-Chalcone Mixture (6:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere $d(A_o)d(A^o)d(A_o)$	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
3.925		13.384	0.6	4483	4483
3.925		12.723	0.6	4716	4716
3.925		12.33	0.6	4866	4866
3.925		11.146	0.6	5383	5383
3.925		10.73	0.6	5592	5592
3.925		10.313	0.6	5818	5818
3.925		10.263	0.6	5846	5846
3.925		10.206	0.6	5879	5879
3.925		10.084	0.6	5950	5950
3.925		9.756	0.6	6150	6150

Second: Measurement of Conductivity and Calculation of Ionic Strength, Activity Coefficient, and Ionic Atmosphere Thickness for CrCl3:

- A mixture of 0.1 ml of chalcone with various volumes of CrCl3 (0.6, 0.5, 0.4, 0.3, 0.2 ml) was prepared. Conductivity was measured over a period, and ionic strength, activity coefficient, and ionic atmosphere thickness were calculated. The results are shown in the tables and figures below:

Table 8: Conductivity Values for CrCl3-Chalcone Mixture (2:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere $d(A_o)d(A^o)d(A_o)$	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
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3.04	9.804	1	10200	10200
3.04	7.491	1	13350	13350
3.04	6.579	1	15200	15200
3.04	6.192	1	16150	16150
3.04	5.9	1	16950	16950
3.04	5.714	1	17500	17500
3.04	5.362	1	18650	18650
3.04	5.076	1	19700	19700
3.04	4.619	1	21650	21650
3.04	4.264	1	23450	23450

Table 9: Conductivity Values for CrCl3-Chalcone Mixture (3:1 Ratio)

Ionic Thickness $d(Ao)d(A^o)d(Ao)$	Atmosphere	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
2.482		12.858	1.5	11666	11666
2.482		10.87	1.5	13800	13800
2.482		10.714	1.5	14000	14000
2.482		9.934	1.5	15100	15100
2.482		8.876	1.5	16900	16900
2.482		8.638	1.5	17366	17366
2.482		8.123	1.5	18466	18466
2.482		7.692	1.5	19500	19500
2.482		7.258	1.5	20666	20666
2.482		7.053	1.5	21266	21266

Table 10: Conductivity Values for CrCl3-Chalcone Mixture (4:1 Ratio)

Ionic Thickness $d(Ao)d(A^o)d(Ao)$	Atmosphere	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
2.15		20.101	2	9950	9950
2.15		17.167	2	11650	11650
2.15		15.936	2	12550	12550
2.15		15.238	2	13125	13125
2.15		14.363	2	13925	13925
2.15		13.536	2	14775	14775
2.15		12.658	2	15800	15800
2.15		12.384	2	16150	16150
2.15		12.066	2	16575	16575
2.15		11.628	2	17200	17200

Table 11: Conductivity Values for CrCl₃-Chalcone Mixture (5:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
1.923		26.539	2.5	9420	9420
1.923		24.606	2.5	10160	10160
1.923		23.234	2.5	10760	10760
1.923		22.242	2.5	11240	11240
1.923		21.222	2.5	11780	11780
1.923		20.695	2.5	12080	12080
1.923		20.096	2.5	12440	12440
1.923		19.41	2.5	12880	12880
1.923		18.491	2.5	13520	13520
1.923		17.832	2.5	14020	14020

Table 12: Conductivity Values for CrCl₃-Chalcone Mixture (6:1 Ratio)

Ionic Thickness $d(A_o)d(A^o)d(A_o)$	Atmosphere	Activity Coefficient $F(\times 10^{-5})F(\times 10^{-5})F(\times 10^{-5})$	Ionic Strength $I(M)I(M)I(M)$	Molar Conductivity $\Lambda\Lambda\Lambda (\mu S)$	Conductivity (μS)
1.755		44.444	3	6750	6750
1.755		34.156	3	8783	8783
1.755		32.432	3	9250	9250
1.755		30.354	3	9883	9883
1.755		29.126	3	10300	10300
1.755		28.037	3	10700	10700
1.755		26.588	3	11283	11283
1.755		25.751	3	11650	11650
1.755		25.751	3	11650	11650
1.755		25.316	3	11850	11850

Discussion and Interpretation of Results:

The molar conductivity of high concentrations of both salts is less than expected despite the presence of a large number of charged ions. This is because increasing the concentration leads to the ions coming closer together, causing the positive ion (+) to approach the negative ion (-) and form what is known as an ion pair, represented as (M+A-). Continuous exchange occurs between the ions of different pairs, with each ion pair having a specific lifetime. The ion pair behaves as an undissociated molecule and does not contribute to carrying the electric current within the solution. As the concentration of ion pairs in the solution increases, the molar

conductivity decreases because part of the electrolyte concentration is bound in ionic clusters incapable of carrying the electric current. The concentration of ion pairs in the electrolyte solution increases as the ion size decreases and its charge increases, and also as the dielectric constant of the medium increases. It refers not to the bare ion size but to its size when associated with solvent molecules, which is usually larger than the bare ion size (20)(21). In the case of chromium chloride, two types of ion pairs can form at high concentrations of these electrolytes: one with the CrCl_3 ion and the solvent, and the other with the positive electrolyte ion in the solution. The presence of these pairs causes the ion to move slowly and creates an effect. Conductivity may increase again with increasing concentration due to the formation of ion triplets in addition to the effect of the ionic atmosphere. These ion pairs and triplets (e.g., $\text{M}+\text{A}-\text{M}+$ or $\text{A}-\text{M}+\text{A}-$) appear as if they carry a single positive or negative charge, respectively, and can conduct electric current in the electrolyte solution (5).

For the CrCl_3 Electrolyte Solution: Trivalent electrolyte solutions at different concentrations have higher conductivity than monovalent electrolytes (KCl) due to the increased charges contributing to conductivity. Conductivity increases with increasing ionic strength but decreases significantly at high concentrations due to internal forces.

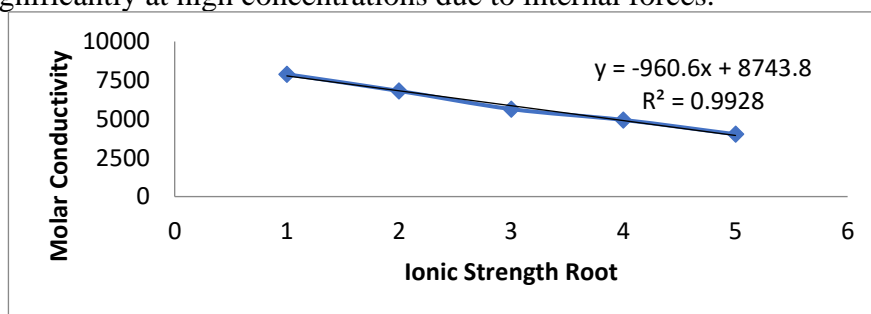


Figure (11): Relationship between Ionic Strength Root and Molar Conductivity for CrCl_3 Salt with Chalcone For CrCl_3 , this relationship and the above plot indicate a negative slope, suggesting that an increase in ionic strength leads to a decrease in molar conductivity and, consequently, a decrease in reaction rate. This occurs in the case of ions with different charges, resulting in a negative slope. The slope value indicates the type of valence ions involved in the reaction, suggesting that one reactant is monovalent and the other divalent, as shown in the following figure.

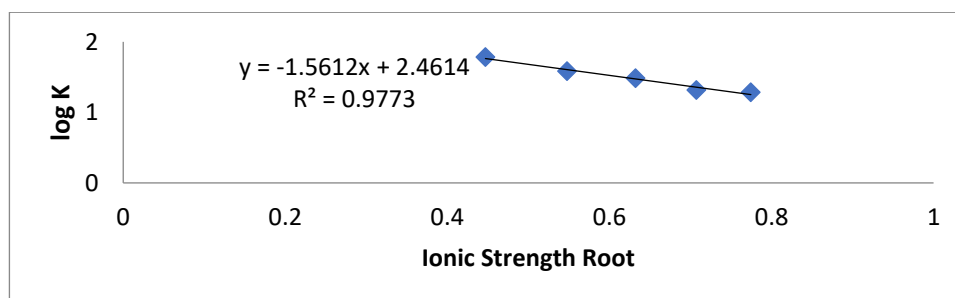


Figure (12): Relationship between Ionic Strength Root and log K for CrCl_3 Salt with Chalcone For KCl salt, as shown in the figure below, the slope value is negative and monovalent, indicating that both reacting ions (chalcone and salt) are monovalent.

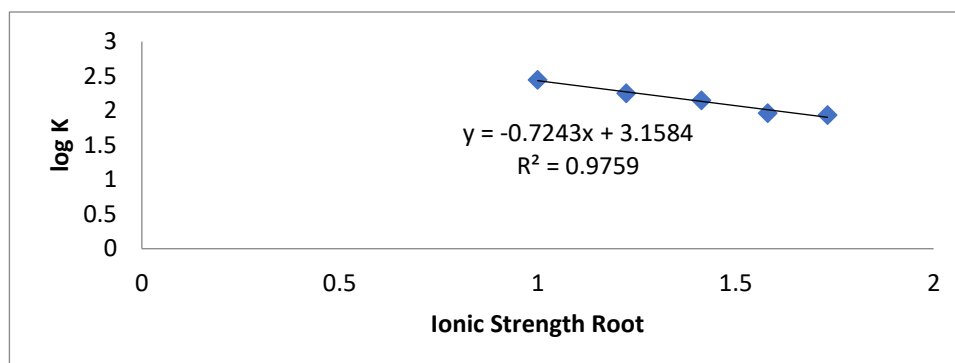


Figure (13): Relationship between Ionic Strength Root and log K for KCl Salt with Chalcone

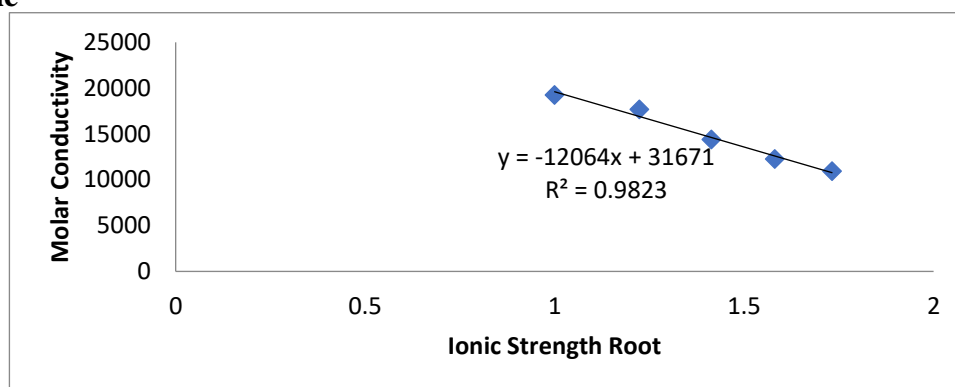


Figure (14): Relationship between Ionic Strength Root and Molar Conductivity for KCl Salt with Chalcone

Conclusions:

- The electrical conductivity (Λ) increases with increasing ionic strength (I) in the order $\text{CrCl}_3 > \text{KCl}$, indicating that trivalent positive ions contribute more to conductivity due to the increased number of current-carrying ions at a given concentration.
- The electrical conductivity (Λ) of the trivalent electrolyte CrCl_3 is higher than that of the monovalent electrolyte KCl due to the increased charges contributing to conductivity, which increases with ionic strength and decreases significantly at high concentrations due to internal forces.
- Activity coefficients (F) for different concentrations were derived from the relationship ($I = F \cdot \text{Cond}$), which can be used to determine ionic strength through direct and easy measurement of electrical conductivity.
- The thickness of the ionic atmosphere was calculated by measuring the electrical conductivity of CrCl_3 and KCl salt solutions in this study using the ionic atmosphere thickness relationship: $d = 4.3 \times [2(F \cdot \text{Cond})]^{-1/2}$

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