Original Research Article

Cyclic Voltammetry Studies for the Interaction of CuCl₂ with 4-Fluoro Benzoic Acid (FBA) in KBr Aqueous Solutions

Esam Arafa Gomaa*, Rania Ramadan Zaky, Mai Samir Nouh

Chemistry Department, Faculty of Science, Mansoura University, Mansoura, Egypt

ARTICLE INFO

ABSTRACT

In this work, cyclic voltammetry studies for Cu (II) ion were carried out to show it`s redox behaviours in 0.1 M KBr and 4-Fluoro benzoic acid. The aim of this research study was to estimate the copper chloride and 4-fluorobenzoic acid in KBr electrolyte. The voltammetric studies involve reversible scans at various concentration of both CuCl₂ and 4-Fluoro benzoic acid (FBA). Based on the measured voltammograms the different thermodynamic parameters such as the Gibbs thermodynamic energies and stability constants for the interaction CuCl₂ with 4-Fluoro benzoic acid (FBA) are discussed by the formation of strong electrostatic complexes. Different Scan rates were also considered to illustrate the mechanism of the redox reactions in the solutions. The importance of this work was to explain the uses of 4-flurobenzoic acid (FBA) as a ligand. Estimation of the different thermodynamic parameters for the interaction of CuCl₂ with 4-flurobenzoic acid in 0.1 M KBr cyclic voltammetry was done. Application of the interaction of CuCl₂ with 4-fluro benzoic acid for evaluation of both different cupprous, cupric and 4-flurobenzoic acid concentrations.

GRAPHICAL ABSTRACT

---
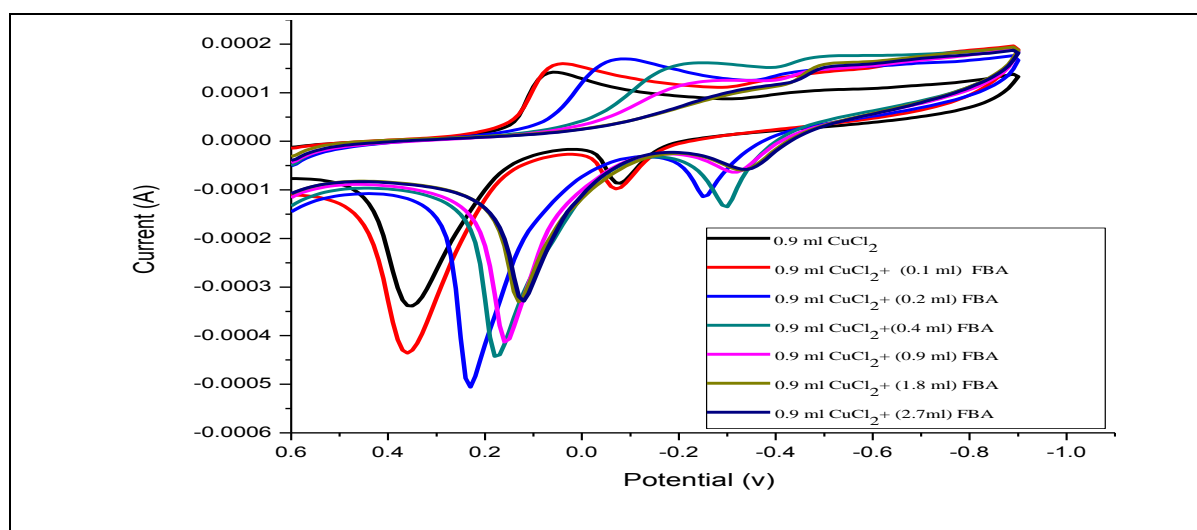
* Corresponding author's E-mail address: eahgomaa65@yahoo.com

Introduction

Cyclic voltammetry is simple, economical technique, which explain the analytical redox reactions for ions under consideration [1, 2]. Copper is a essential metal for animals and plants [3], which combined with ligands forming complexes of vital biological effect [4]. Synthesis of complexes with low molecular weight is the target for many researchers for bioinorganic chemistry for obtaining high catalytic activity compounds [5, 6]. The aim of the work was to estimate both the copper chloride and fluorobenzoic acid in aqueous electrolyte. Also the use of 4-furobenzoic acid as ligand for compleximg with copper to facilitate its determination.

Inorganic elements such as Cu is not created or disappeared, therefore must be under the control [7-12]. One property of Cu that its diverse roles in structure and catalysis and its existence in either a reduced Cu^+ or oxidized Cu^{++}. Cu^+ has affinity for thiol and thioether group and Cu^{++} exhibits preferred coordination to oxygen and imidazole nitrogen groups found in glutamic, aspartic acid and histidine. The process of change between Cu^+ and Cu^{++}, free intracellar Cu can generates hydroxyl radical which can damage the proteins, nucleic acids, and lipids. Also it can interfere with the synthesis of Fe-sulfur clusters that are essential for the activity of number of cellular enzymes. In addition Irving-Williams predicted that Cu can displace other metals such as Zn from their cognate in metalloproteine, resulting in inappropriate protein structure and interrupt, enhibit enzymatic activity [19-12]. Therefore copper estimation in all its forms is essential to detect them and may increase the intensity of peaks by using simple ligand like 4-fluro benzic acid. On giving 4-flurobenzoic acid to patiants as

drug in small amounts can form compelex with copper ions and then analytically determine them in serum. Cyclic voltammetry gives advantages over other techniques as it is rapid, easy method and permit the different analytical parameters. In this work, cyclic voltammetry was employed to assess the electrochemical behavior of Cu (II), 4-Fluoro benzoic acid (FBA) in aqueous 0.1 M KBr [13-17].

Experimental

Materials and methods

The copper chloride and potassium bromide used in this study were purchased from the Sigma Aldrich. All chemicals were used without purification. Deionized pure water was used. The systematic cell consists of group of three electrodes connected to pot state of the type DY 2 0 0 0. The first electrode silver-silver chloride filled with saturated KCl was employed as reference electrode. The second electrode was glassy carbon electrode (GCWE) which preared in our laboratory from pure carbon pease jointed to copper wire and then isolated by heat shrink polymer to prevent contacting with the solutions, this electrode was purified by polishing with aluminium oxide and wool pease till mirror was formed then clearly washed with distilled water many times. Third electrode was a counter electrode of platinum (Pt). Flow of N_2 gas was partialized to bring inert atmosphere. Area of electrode was 0.502 cm². The glassy carbon working electrode (GCWE) was polished till shiny black mirror appearred. Fresh solutions of $CuCl_2$, KBr and 4-fluoro benzoic acid (FBA) were prepared. All the experiments were done at 19.7 °C.

Theoretical calculations

Figure 1. Gaussian 09 3D Structure of 4-fluoro benzoic acid
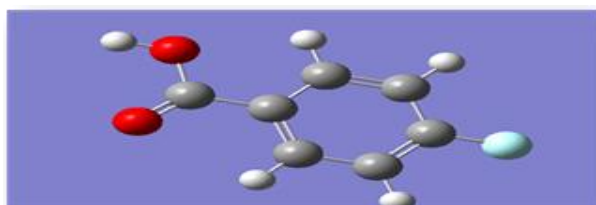
Results and discussion

The electrochemical manner of CuCl₂ in KBr (0.1 M) in absence of 4-Fluoro benzoic acid (FBA)

The physicochemical behaviour of $CuCl_2$ solution in KBr (0.1 M) at 292.85 K in absence of 4-Fluorobenzoic acid (FBA) was studied at potential window of 600-900 mV.

Effect of change of CuCl₂ concentration

Increasing of anodic and cathodic peak height accompanied with slight shifting in voltage, to more positive by raising the concentration of $CuCl_2$ via adding different concentrations of $CuCl_2$ (0.002, 0.0023, 0.0027 and 0.003M) in KBr (0.1 M) at sampling frequency (0.1 v/s) as shown in Figure 2, which can be clarified by appearance of a massive number of electroactive species in solution [7,8]. By plotting a relation among different concentration of metal salt and current we get a linear relation with a linear correlation (r^2 =0.93), this increase may give indication of that system is diffusion controlled [9,10].

Impact of changing scan rate of CuCl₂

The scan rate ranging from 10 to 100 mv/s was applied to evaluate the physicochemical action of copper ions in solution (Figure 4). Raising of sampling frequency rate was followed by increasing the ks, Γ(a), Γ(c), and favoring the diffusion processes. The linear change for the anodic and cathodic peak current against root mean square of potential scan rate in Figure 5 indicates the diffusion control of the $CuCl_2$ in KCl solution.

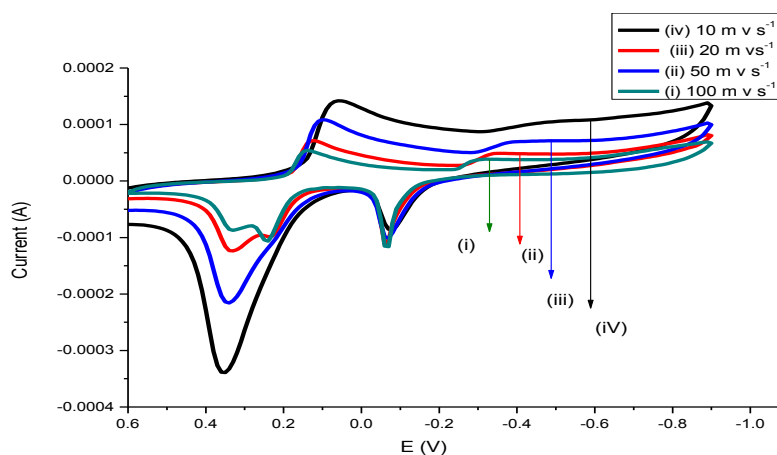**Figure 2.** Cyclic voltammograms of different concentrations of CuCl₂ in 0.1 M KBr (I) 00.0023 M, (II) 00.0027 M and (III) 00.0030 M
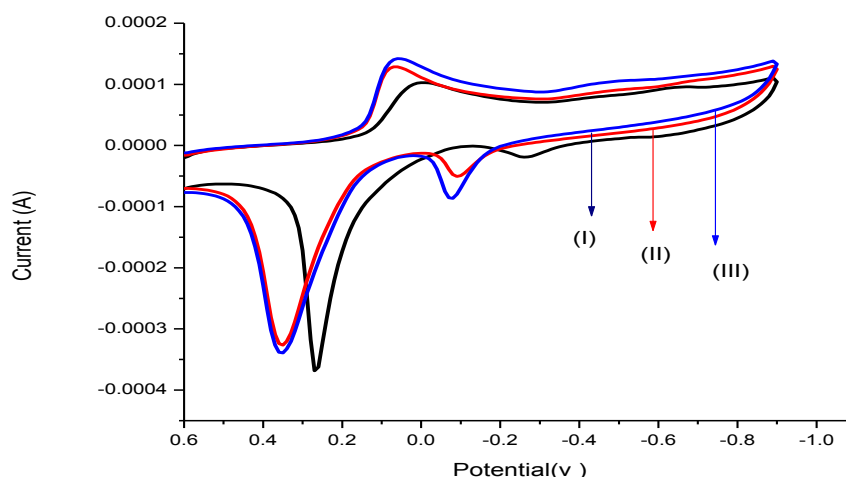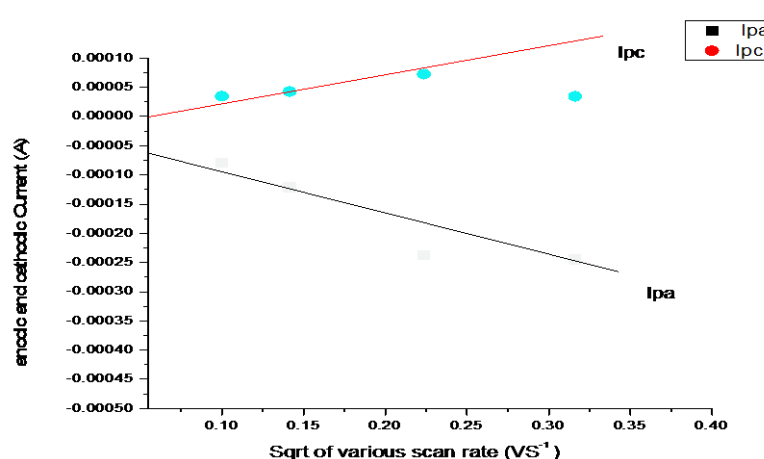

Figure 3. Anodic peak current against concentration of CuCl₂ within KBr (0.1 M)
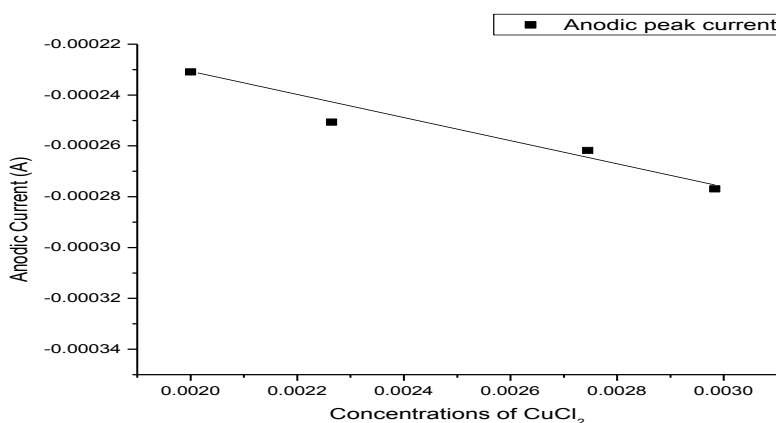
Figure 4. Cyclic voltammetry behaviors of 1 mM CuCl2 in 0.1 M KBr at various scan rates

Figure 5. Cathodic and anodic current denisity against square root of different sampling frequancy for 1 mM CuCl$_2$

Table 1. Voltammetric parameters of CuCl$_2$ (1 mM) in absence of 4-Flourubenzoic acid (FBA) at various scan rate in KBr (0.1 M) at 19.7 °

Scan rate (v/ s)	$\nu^{1/2}$	[M] (mol. L^{-1})	(-) Ipa * 10^{-04} (mA)	Ip$_c$*10^{-05} (mA)	Ip$_a$/Ip$_c$	E$_{Pa}$ (v)	E$_{pc}$ (v)	ΔEp (v)	E ½ (v)
0.1	0.3162	0.003	2.51	7.46	3.3626	0.3514	0.0563	0.2952	0.2039
0.05	0.2236	0.003	1.49	7.75	1.9259	0.3320	0.0978	0.2342	0.2149
0.02	0.1414	0.003	1.04	6.04	1.7206	0.3216	0.1090	0.2126	0.2153
0.01	0.1000	0.003	0.648	4.44	1.4600	0.2737	0.1345	0.1392	0.2041

Table 1 illustrates the cathodic and anodic peak current, the peak potentials, peak potentials separation and peak current ratios at all various sampling frequency rate through the study of behavior of 1 mM of CuCl$_2$.

The scan effect parameters for 0.003 M CuCl$_2$, anodic diffusion constant Da, cathodic diffusion constant Da, heterogeneous rate constant ks, anodic surface coverage Γa, cathodic surface coverage Γa, anodic quantity of electricity Qa in Columb unit (C), cathodic quantity Qc of electricity are increased by increase in the scan rate for CuCl$_2$ solution indicating the diffusion control redox mechanism.

Figure 6. Anodic peak current of the first oxidation peak against scan rate for cyclic voltammograms of 1 mM of CuCl$_2$
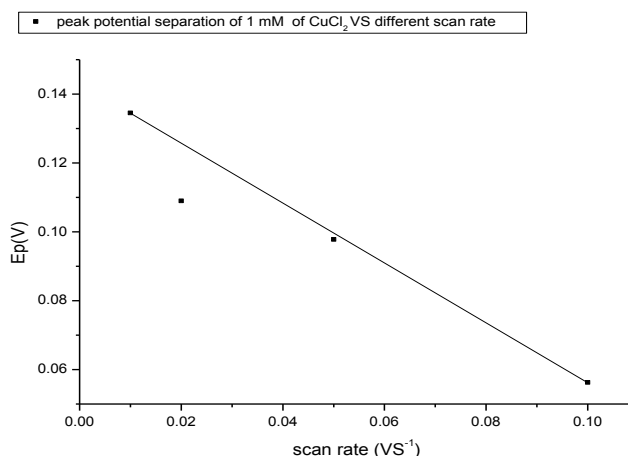
Table 2. Effect of different scan rates of 0.003 M CuCl$_2$ at 19.7 °C on the diffusion parameters Electronic structure

Scan rate (vs^{-1})	$\nu^{1/2}$	[M] (mol. L^{-1})	Da (cm^{2}s^{-1})	Dc (cm^{2}s^{-1})	log ks (cm.s^{-1})	Гax10^7 (mol.cm^2)	Гc (mol.cm^2)	Qa * 10^{-8} (C)	Qc (C)
0.1	0.3162	0.003	0.4961	0.0439	152.5701	1.4521	0.0013	4.3184	0.0004
0.05	0.2236	0.003	0.1757	0.0474	95.8016	1.0887	0.0013	5.6527	0.0007
0.02	0.1414	0.003	0.0537	0.0537	78.7310	1.5607	0.0020	9.0709	0.0012
0.01	0.1000	0.003	0.0347	0.0163	33.0200	0.8342	0.0016	5.7139	0.0011

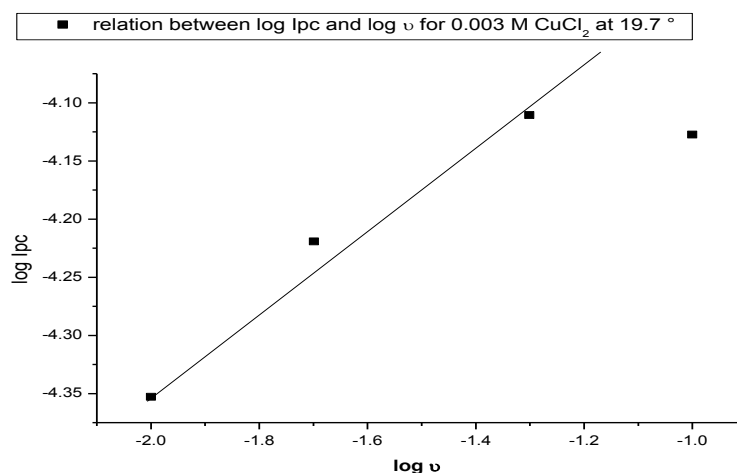**Figure 7.** log Ipc and log ν for 0.003 M CuCl$_2$ at 19.7 °

Figure 7, illustrates the relation between the log Ip and log ν (the linear plot), indicating that the mechanism was diffusion controlled for 0.003 M CuCl$_2$ immersed in 0.1 M KBr. Increasing the linearity is a sign of the irreversible manner of the electrochemical reactions [11]. Randles Sevicek formula [21-20] was used to make a relation between the peak currents (anodic and cathodic).

Electrochemical manner of Copper Chloride CuCl$_2$

in presence of 4-Flouro benzoic acid in 0.1 M KBr Solution

Effect of ligand concentration

Voltametric behaviour of Copper ions in the existence of 4-Flouro benzoic acid (FBA) in KBr (0.1 M) at a certain temperature (292.85 K) have been investigated from 600: 900 mv voltage ranging. Cyclic voltammograms in Figure 8 illustrate the electrochemical behavior of complex interactions between CuCl$_2$ and 4-Fluoro-benzoic acid (FBA) in 0.1M KBr

supporting electrolyte for anodic from 489: 545 mv and moving slightly in cathodic peak potential from 41: 76.9 mV.

The reduction mechanism of the $CuCl_2$ alone gave two reduction peaks at approximately -0.2 and -0.5 V corresponding to the reduction of divalent cupric ion to monovalent one and the second peak is the reduction of monovalent cuprous ion to zerovalent one (copper metal).

The corresponding oxidation peaks happened in the opposite direction with two peaks ant -0.4 and +0.1 V approximately corresponding to the oxidation of zerovalent copper to monovalent cuprous ion and the second peak is the oxidation of cuprous to cupric ion consumuing one electron in each step [21]. On adding 4-flurobenzoic acid to $CuCl_2$ solution in 0.1 M KBr positive shift in the

reduction peaks was happened firstly and then negative shift followed due to the interaction between 4-flurobenzoic acid and $CuCl_2$ by association and complexation mechanism,the complexation is supported also by positive shift in the oxidation peaks [21]. The oxidation peaks of $CuCl_2$ were shifted mostly to more positive values indicting the compexation charater is explained here by the oxidation peaks. Cyclic voltammetry behavior of different concentrations of the copper ions were examined at the steady state and the hemicycle waves were analyzed using the Randles-Sevcik equation (Equation 1). A range of scan rate (10 to 100 mv/s) was studied to follow the redox mechanism for copper ions alone. Different cyclic voltammetry data of the analysis of the cyclic voltammograms diagrams were obtained.

Figure 8. Cyclic voltammograms for interaction of 1mM of $CuCl_2$ in presence of 1mM 4-Flouro benzoic acid(FBA)
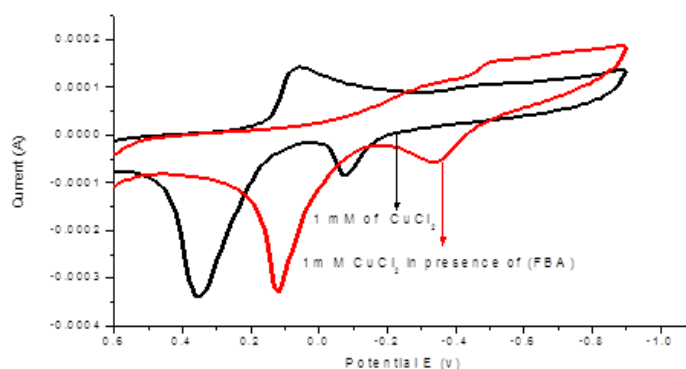
Figure 9. Cyclic voltammograms for interaction of $CuCl_2$ with different Concentration of 4-Flouro benzoic acid in 0.1 M KBr Solution
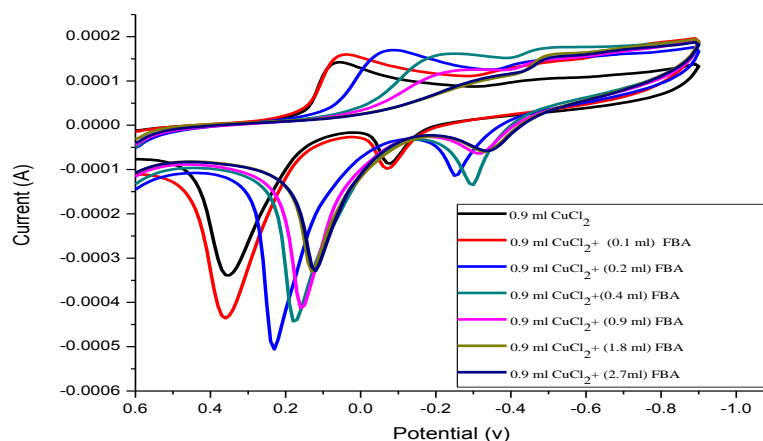
Cyclic voltage behavior of different concentrations of copper ions were examined at the steady state and the hemicycle waves were analyzed using Randles-Sevcik equation (1).

$$I_p = (2.69 * 10^5) \, n^{3/2} \, A \, C \, D^{1/2} \, \nu^{1/2} \qquad (1)$$

Where (I_{Pa}) is anodic current, (I_{pc}) symbol for cathodic current, (ΔEp) refers to potentials difference, (Da) diffusion factor for anode, and (D_C) diffusion factor for cathode. (ks) diffusion rate for electrons, ($\Gamma(a)$) surface coverage, (C) cathodic area coverage, (qa) anodic quantity of electricity, (α na) is the transfer coefficient. Quasi reversible reactions were observed for the redox behavior of the $CuCl_2$ in 0.1 M KBr at 19.7 °C. All the cyclic voltammetry parameters that calculated from the cyclic voltammograms indicated their increase in all values favoring increase in the diffusion-controlled parameters. The used and applied equations for electrochemical analysis are [12-15].

$$Ip = 0.4463 n^{3/2} F^{3/2} D^{1/2} Ac\nu^{1/2} /RT^{1/2} \qquad (2)$$

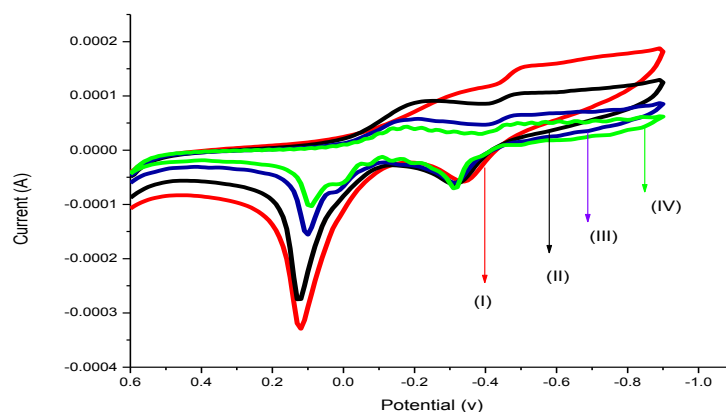$$D^{3/2}(slope, Ip \, \nu^{1/2})(RT)^{1/2}/(0.4463 \, \nu^{3/2}F^{3/2}AC \quad (3)$$

$$\Delta Ep = Ep, a - Ep, c = 2.303 \, RT/nF \qquad (4)$$

$$\Psi = \gamma^a \, k_s/(\pi_a\nu D_a)_{1/2} \qquad (5)$$

$$\gamma = Da^{1/2}/Dc^{1/2} \qquad (6)$$

$$a = nF/RT \qquad (7)$$

Where (Ψ) is the charge transfer which approximately equal one [16], Gas constant (R), absolute temperature (T) under study (a) was taken to be 0.5 which used for approximation for calculations, Area for electrode (A). Voltammetric study for the interaction of $CuCl_2$ with 4-Fluorobenzoic acid (FBA) by different addition of concentrations (FBA) on 1mM $CuCl_2$ was investigated at (GCWE) within voltage range of 0.041 to 0.0769 addition of 4-Fluoro benzoic acid were done till 1:1 (M/L) (Metal, ligand, Matrix).Forming 1:1 complex ($CuCl_2$: FBA) includes the voltage shift to more negative values in the forward direction through two reduction waves and less negative values for reverse sweep for the oxidation peaks.

Effect of different scan rate of complex

Impact of scan rate on the interaction among $CuCl_2$ in presence of 4-Flouro benzoic acid in 0.1 M KBr Solution was studied in 10, 50, 20 and, 100 mv/s are demonstrated in Figure 10. Cathodic (Ep, c) and anodic (Ep, a) wave potentials, peak current (Ip, i) and the peak current ratio (Ipa/Ipc) and separation between the two potentials ΔEp were obtained (Table 3). By enhancing the scan rate for the complex ($CuCl_2$/FBA), the anodic and cathodic wave current increased, anodic peaks voltage shifted to more positive value and the cathodic peak voltage were shifted towards negative values. These founding suggest diffusion controlled at GCWE.

Figure 10. Different scan rates (I) 10 mv, (II) 50 mv, (III)20 mv and (IV) 100 mv of complex 0.003 M $CuCl_2$ interacted with 0.00075 M
4-Flouro benzoic acid (FBA) in 0.1 M KBr at 19.7 °C

The complex stability constants (B) for interaction of $CuCl_2$ with 4-Fluoro benzoic acid (FBA) in 0.1 M KBr were determined by using equation (8) [16-25].

$$(Ep)M-(Ep)c=2.303RT/nF \log \beta_C + 2.303RT/nF \log(C) \qquad (8)$$

Where $(Ep)_M$ is the peak voltage for $CuCl_2$ without adding (FBA). $(E_P)_C$ is peak voltage of the formed complex, R gas constant, (C) is the concentration for used ligand 4-Flouro benzoic acid. Gibbs free energies of interaction of $CuCl_2$ with FBA were evaluated by using equation (9) [25-39].

$$\Delta G=-2.303RT \log \beta_C \qquad (9)$$

The impact of 4-Flouro benzoic acid on $CuCl_2$ is explained by thermodynamic parameters as β_C and ΔG which presented in Table 3. For 1:1 stoichiometric complex, we estimate the thermodynamic parameters for various frequencies as shown in Table 4.

All the cyclic voltammetric data given in Table 3 like anodic potential Epa, cathodic potential Epc, anodic current Ipa, cathodic peak current Ipc, difference in potentials Ipa/Ipc and the relation between anodic current to cathodic current Ipa/Ipc are increased by increase in the scan rate indicating the diffusion contol of our reaction mechanism.

The thermodynamic functions, stability constants β_C and Gibbs free energies ΔG of interaction between $CuCl_2$ and 4-flurobenzoic (FBA) acid given in Table 4 indicate the interaction between them firstly strong and then decrease by more adding 4-flurobenzoic acid (FBA) due to the little places found available for complexation.

The different energy parameters like correction to zero point, energy thermal correction, enthalpy thermal correction, thermal correction to Gibbs free energy, sum of zero-point energies electronic energy, sum of thermal energies and electronic, sum of thermal ethapies, electronic and sum of electronic and thermal free energies are great detectable quantity in Hartree (1 Hartree X627.50 = k.cal/mol) indicating the activity of 4-flurobenzoic acid (FBA) as ligand.

Table 3. Voltammetric parameters of various scan rate of 1 mM $CuCl_2$ in presence of 1 mM 4-Flouro benzoic acid (FBA) in KBr (0.1 M) Solution

ν (v.s⁻¹)	ν ^(1/2)	Epa (v)	- Epc (v)	- Ipa *10⁻⁴	Ipc*10⁻⁵ (A)	ΔEp (v)	Ipa / Ipc
0.1	0.3162	0.1226	0.5184	2.45	3.23	0.6409	7.5714
0.05	0.2236	-0.3019	0.2207	4.23	7.24	-0.0812	5.8416
0.02	0.1414	0.1018	0.1784	1.21	4.27	0.2802	2.8378
0.01	0.1000	0.0958	0.1747	0.795	3.48	0.2704	2.2857

Table 4. Solvation parameter of the interaction among $CuCl_2$ and 4-Flouro benzoic acid (FBA) at 19.7 ºC

T K	ml added of ligand	[L] (Mol.L⁻¹)	E ½ C (V)	E ½ M (V)	ΔE ½ (V)	log β_C	ΔG (KJ)
292.85	0.1	0.00003	0.2033	0.2039	0.0006	4.5661	-25.6033
292.85	0.2	0.00006	0.0826	0.2039	0.1213	6.3422	-35.5625
292.85	0.4	0.00011	0.2057	0.2039	0.0018	3.9857	-22.3489
292.85	0.6	0.00017	0.2082	0.2039	0.0044	3.8534	-21.6068
292.85	0.9	0.00025	-0.0266	0.2039	0.2305	3.640	-20.411
292.85	1.8	0.00050	-0.1869	0.2039	-0.3908	3.4246	-19.2023
292.85	2.7	0.00075	-0.1894	0.2039	-0.3933	3.6438	-20.4317

Table 5. Gaussian 09 statistical thermodynamic calculations for 4-Flouro benzoic acid (FBA) in ethanol including entropy S, heat capacity at constant volume CV, total energies, individual energies and partition functions Q

Correction of zero-point	0.110950 (Hartree/Particle)	
Energy thermal correction	0.119193	
Enthalpy thermal correction	0.120137	
Thermal correction to Gibbs Free Energy	0.074802	
Sum of zero-point Energies and electronic	-0.064662	
Sum of thermal Energies and electronic	-0.056419	
Sum of thermal Enthalpies and electronic	-0.0554755	
Sum of electronic and thermal Free Energies	-0.100810	
	$E_{thermal}$ k/cal/mol	CV cal/mol-kelvin	S cal/mol-kelvin
Total	74.795	29.824	95.415
Electronic	0.000	0.000	0.000
Translational	0.899	2.982	40.723
Rotational	0.899	2.982	29.504
Vibrational	73.017	23.863	25.190
Vibration 1	0.593	1.987	8.863
	Q		
Total V=0	0.423438D+17		
Vib (Bot)	0.962255D-48		
Vib (B0t) 1	0.318150D+02		
Vib (V=0)	0.103890D+04		
Vib (V=0) 1	0.323189D+02		
Electronic	0.1000000D+01		
Translational	0.651290D+08		
Rotational	0.625809D+06		

The different statistical thermodynamic parameters, thermal energy E thermal. Heat capacity at constant volume CV and entropies of the solvation of (FBA) in ethanol gave data shown in Table 5 indicate that vibrational statistical thermodynamic parameters are valuable values favouring activity of 4-flurobenzoic acid (FBA). This is supported by the partiton functions of 4-furobenzoic acid (FBA) given also in Table 5 with high electronic, translational and rotational partition Q functions.

Conclusion

The cyclic voltammetry of CuCl₂ alone gave two reduction and two oxidation peaks in 0.1 M KBr solutions. On adding 4-furobenzoic acid (FBA) interaction between the two decreased the currents of the four redox waves and shift in the potentials of the peaks.The different cyclic voltammetry parameters were estimated to explain the redox behavior of CuCl₂ in 0.1 M KBr in absence and presence of 4-flurobenzoic acid (FBA). The activity of 4-furobenzoic acid was proved from theoretical quantum chemistry calculation using Gaussian 09 set programs and cyclic voltammetry measurements.The thermdynmic parameters estimated for the interaction of CuCl₂ with 4-flurobenzoic acid (FBA) like the stability constant and Gibbs free energy of interaction gave good data indicate the association and the complexation of CuCl₂ with 4-flurobenzoic acid forming aqueous complex reaching (ΔG=-35 kJ as maximum value).

Acknowledgement

We gratefully acknowledge staff members and head of Chemistry Department in Faculty of Science, Mansoura University for their help.

Disclosure statement

No potential conflict of interest was reported by the authors.

References

[1] S. Nagalingam, G. B. Teh, *Scientif. study Res.*, **2014**, *15*, 1–7.

[2] J.L. Anderson, L. Shain, *Anal. Chem.*, **1976**, *48*, 1274–1282.

[3] J. Becker, D. Brockway, K.S. Murray, P. Newman, T. Toftlund, *Inorg. Chem.*, **1982**, *21*, 1791–1798.

[4] R.N. Patel, *Spectrochim. Acta, A,* **2003**, *59*, 713–721.

[5] I. Ibarrolla, M.C. Arilla, M.D.Herrero, M.I. Esteban, A. Martinez, J.A. Asturias, *J. Invest. Allergol. Clin. Immunol.*, **2008** , *18*, 78–83.

[6] E.C. Ukpong, *Int. J. Eng. Sci.*, **2013**, *2*, 1–13.

[7] A.K. Boal, A.C. Rosonzweig, *Chem. Rev.*, **2009**, *109*, 4760–4779.

[8] B.E. Kim, T. Nevitt, D.J. Thiele, *Nat. Chem. Biol.*, **2008**, *4*, 176–185.

[9] S. Lutsenko, *Curr. Opin. Chem. Biol.*, **2010**, *14*, 211–217.

[10] Y. Nose, B.E. Kim, D.J. Thiele, *Cell. Metab.*, **2006,** *4*, 235-244.

[11] S. Punig, N.U.R. Andres-Colas, A.N.T. Garacia-Molina, L. Penarrubia, Plant *Cell Environ.*, **2007**, *30*, 271–290.

[12] C. White, J. Lee, T. Kambe, K. Fritsche, M.J. Petris, *J. Biol. Chem.*, **2009,** *284*, 33949–33956.

[13] M. Eldefrawy, E.A. Gomaa, S. Salem, F. Abdel Razik, *Prog. Chem. Biochem. Res.,* **2018**, *1*, 11–18.

[14] A. Taheri, R. Faramarzi, M. Roushani, *Anal. Bioanal. Electrochem.*, **2007**, *7*, 666–683.

[15] G. Vinodhkumar, R. Ramya, M. Vimalan, I. Potheher, A. Cyrac Peter, *Prog. Chem. Biochem. Res.*, **2018**, *1*, 40–49.

[16] Rezayati-Zad Z., Davarani S.S.H., Faheri A., Bide Y., *Biosens. Bioelectron.,* **2016**, *86*, 616–622.

[17] S. Mohammadi, A. Taheri, Rezyati-Zad Z., *Prog. Chem. Biochem. Res.*, **2018**, *1*, 1–10.

[18] R.S. Nichiolson, I. Shain, *Anal. Chem.*, **1964**, *36*, 706–723.

[19] T.S. Anirudhan, F. Shainy, J.R. Deepa, Chem. Ecol.**, 2019**, *35*, 235–255.

[20] A.M. El-Askalany, A.M. Abou El-Magd, *Chem. Pharm. Bull.*, **1995**, *43*, 1791–1792.

[21] E.A. Gomaa, M.A. Morsi, A.E. Negm, Y.A. Sherif, *Int. J. Nano Dimens.*, **2017**, *8*, 89–96.

[22] C.P. Kelly, C.J. Cramer, D.G. Truhlar, *J. Phys. Chem. B.*, **2006**, *110*, 16066–16081.

[23] M.A. Morsi, E.A. Gomaa, A.S. Nageb, *Asian J. Nanosci. Mater.*, **2018**, *1*, 282–293

[24] S. Magdassi, M. Grouchko, A. Kamyshny, *Materials*, **2010**, *3,* 4626–4638.

[25] A.K. Chatterjee, R. Chakraborty, T. Basu, *Nanotechnology*, **2014,** *25*, 135101.

[26] O. Gutten, L. Rulíšek, *Inorg. Chem.*, **2013**, *52*, 10347–10355.

[27] J.I. Kim, A. Cecal, H.J. Born, E.A. Gomaa, *Z. Phys. Chem.*, **1978**, *110*, 209–227

[28] J.I. Kim, E.A. Gomaa, *Bull. Soc. Chim. Belg.*, **1981**, *90*, 391–407

[29] F.I. El-Dossoki, E.A.Gomaa, O.K. Hamza, *J. Chem. Eng. Data*, **2019**, *64*, 4482–4492

[30] S. Eloul, R.G. Compton, *J. Phys. Chem. C*, **2015**, *119*, 27540–27549.

[31] K.M. Ibrahim, E.A. Gomaa, R.R. Zaky, M.N. Abdel El-Hady, *Am. J. Chem.*, **2012**, *2*, 23–26.

[32] E.A. Gomaa, *Int. J. Mater. Chem.*, **2012**, *2*, 16–18.

[33] E.A. Gomaa, *Phys. Chem. Liq.,* **2012**, *50*, 279–283.

[34] E.A. Gomaa, *Am. J. Environ. Eng.,* **2012**, *2*, 54–57.

[35] M.N. Abd Elhady, E.A. Gomaa, A.G, Al-Harazie, *J. Mol. Liq.*, **2019**, *276*, 970–985.

[36] E.A. Gomaa, A. Negm, R.M. Abu Qarn, *Iran. J. Chem. Eng.*, **2017**, *14*, 90–99.

[37] E.A. Gomaa, *Int. J. Theor. Math. Phys.,* **2013**, *3*, 151–154.

[38] E.A. Gomaa, *Indian J. Tech.*, **1986**, *24*, 725–726.

[39] E.A. Gomaa, G.M. Beghit, *Asian J. Chem.*, **1990**, *2*, 444–450.