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Cyclic Voltammetry for Interaction between Mercuric Chloride and Diamond Fuchsin (Rosaniline) in 0.05 M NaClO₄ Aqueous Solutions at 303 K

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ABSTRACT

The cyclic voltammetry of different concentrations of mercuric chloride in 0.05 M NaClO₄ as a supporting electrolyte was studied in the absence and presence of diamond fuchsin as magneto dye at K using a glassy carbon electrode as the working electrode. The effects of scan speeds (rate) were also studied, and the evaluated data were discussed. Diamond Fuchsin (rosaniline hydrochloride) magneto dye was used as a complexion material. The different solvation, kinetic, and thermodynamic parameters were evaluated from the cyclic voltammograms and found weak interaction between the magneto dve used and mercuric ions. Mercuric chloride can undergo redox reactions and studying its cyclic voltammetry provide insights into its electrochemical properties and have some potential important uses, like, sensor development and toxic estimation in environmental monitoring and electroplating studies. Safety guidelines should be considered by cyclic voltammatery to follow the toxic mercuric ions. The main target is to estimate the qualitative and quantitative concentration of very toxic mercuric ions as safely and fast.

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Introduction

Voltammetry is the application of a potential waveform for further study of the behavior of a species in solution. It provides information about the electrochemical properties of a substance, such as oxidation and reduction potentials, diffusion coefficients, and electron transfer kinetics [1-10]. Mercuric ions have many applications in various fields. Firstly, an evaluation of the redox behavior of mercuric ions can provide insights into the stability and interaction of the used materials. Secondly, important characterizations for mercuric ions can be estimated. Thirdly, environmental monitoring of the toxicity of mercuric chloride, using cyclic voltammetry as sensors for mercuric ion evaluation, and then materials science is used to investigate the interaction of mercuric ions with other compounds. This work is the continuation of our previous work published in the *Chemical* Methodologies Journal to gain new novel data about the very toxic mercuric ions [11, 12].Cyclic voltammetry can be used to estimate various parameters related to mercuric chloride, such as its redox potential, diffusion coefficient, and concentration by analyzing the shape and position

of the voltammograms which can be useful for understanding its reactivity and stability. Cyclic voltammetry can be used to detect and quantify mercuric chloride in environmental samples, helping in monitoring its presence. Electrode material characterization can be obtained from cyclic voltammetry which provide insights into the electrochemical behavior. The benefits of the use of cyclic voltammetry are the sensitivity is a highly sensitive technique. Selectivity of redox behavior can be studied by cyclic voltammetry allowing for selective detection. Rapid analysis cyclic voltammetry was studied here. Versatility of measured cyclic voltammograms was examined under various experimental conditions [7-12].

Overall, Cyclic voltammetry offers a powerful approach to investigate the electrochemical properties of mercuric chloride and has numerous applications in environmental monitoring, material characterization and analytical New applications chemistry. for cvclic voltammetry as using Silver nanoparticles decorated functionalized multi-walled carbon nanotubes modified screen printed as a sensor for the voltammetric determination of butorphanol [13].Recent work in cyclic voltammetry is preparation of new electrochemical sensor for the ketoconazole detection using carbon paste

electrode modified with sheaf-like Ce-BTC MOF nanostructure and ionic liquid [14]. New work about voltammetric determination of hydrochlorothiazide at a modified carbon paste electrode with polypyrrole nanotubes was done [15]. New voltammetric determination of vitamin B6 in the presence of vitamin C based on zinc ferrite nanoparticles modified screen-printed graphite electrode was done recently [16]. Application of electrochemical sensor for determination of butylated hydroxyanisole in real samples using glassy carbon electrode modified by [Co(HL)₂Cl₂] nano-complex application was done [17]. $CuFe_2O_4$ nanoparticles-based was

prepared as electrochemical sensor for sensitive determination of anti-cancer drug 5-fluorouracil [18].

Materials and Method

Pure Mercuric chloride (HgCl₂) from Merck Company was used in the present study, diamond fuchsin from Riedel De Haen AG Germany was used as ligand, pure NaClO₄ was prepared from perchloric acid and sodium hydroxide, as presented in previous sudies [13,14] as a supporting electrolyte and all experiments were done using deionizer water.

Name	Mercuric Chloride	Diamond Fuchsin (As a disinfectant)	Sodium perchlorate
Structure	Cl Hg Cl	H ₂ N NH ₂ ⁺ Cl ⁻	O ⁻ Na ⁺ O=Cl=O ∥ O
Formula	HgCl ₂	C ₂₀ H ₁₉ N ₃ ·HCl	NaClO ₄
Molar Mass	271.52 g/mol	337.86 g/mol	122.4 g/mol

Cyclic voltammetric analysis (CV)

DY2000 multichannel potentiometer was used and applied origin for further analytical data.

Results and Discussion

Electrochemical behavior of mercuric chloride alone at 303 K

Mercuric ion concentrations effect

First, a cyclic voltammogram of 30 ml NaClO₄ (0.05) M as a supporting electrolyte was measured in the range (2 to -2) V at 303 K (Figure 1 (a and b)), original and calculated, and then the redox behavior of mercuric ions was examined in 30 ml NaClO₄ (0.05) M at 03 K. The mercuric chloride solution HgCl₂ is added stepwise from 3.31×10^{-4} M to reach 13.0×10^{-4} M, as displayed in Figure 1.

The redox mechanism of the used mercuric chloride is happened through two electron

mechansim for the reduction of Hg²⁺ to mercury zero, and the oxidation is the opposite of both stages. The waves are at 0.15 and -0.15 V for the reduction peaks, which explain the mercuric ion reduction by interaction with two electrons, forming the mercurous ion first, and this step is followed by the reduction of mercurous to metal mercury with valence zero. For the oxidation, two oxidation peaks appear at 0.33 and 0.73 V, which are the opposite waves of the reduction one. For further study, we chose the initial reduction wave with the first oxidation peak for different analyses. Two electrons are consumed for the redox reaction of mercuric chloride in 0.05 M NaClO₄. We follow the second electron transfer in the reduction and the initial dissolution wave of the deposited mercury.

Analysis of the obtained voltammograms were done following equations given is literature references [14-22]. Checking the reversibility degree was also done, following the other references [15, 16].

The calculated solvation and kinetic parameters of lead ions at 302.15 K and a scan rate of 0.1 V/S are presented in Table 1. All the equations used for analyzing the waves are given and explained in different and previous references [15-30]. Most of

the analysis data for different concentrations of mercuric chloride are increased by increase in mercuric ion concentrations supporting the diffusion mechanism, especially the adsorption solvation data like the cathodic Γ_{c_n} anodic surface coverage Γ_a , anodic Q_a , and cathodic quantity of electricity, as presented in Table 2.



Figure 1: Cyclic voltammetry of HgCl₂ in NaClO₄ (drawn from origin program) and the original cyclic voltammograms are given at the right side

Fable 1: The Cyclic voltammetry parameters $[\Delta Ep$, Da.	<i>Dc</i> α_{nc} , k_{s} , Γ_{a} , Γ_{c} , and Q_{c}] of HgCl ₂ in 0.05 (mole.dm ⁻³) NaC	2 10 4
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[HgCl2] x10-4	E _{pa} (V)	(-)E _{pc} (V)	(-)I _{Pa} µA	Ι _{Ρc} μΑ	D _a x10 ⁻¹⁰ cm ² .s ⁻¹	D _c x10 ⁻¹⁰ cm ² .S ⁻¹	(-)Ep _{c/2} V	αna	k _s x10 ⁻² cm.s ⁻¹	Γ _c x10-9 mol/cm ²	Q _c x10 ⁻⁵ Coulomb	Γ _a x10-9 mol/cm ²	Q _a x10 ⁻⁵ Coulomb
3.31	0.207	0.167	2.18	3.29	1.538	3.50	-0.16	6.10	19.2	5.63	3.41	3.73	2.26
6.58	0.307	0.118	5.51	4.37	2.489	1.57	-0.05	0.70	11.6	7.48	4.54	9.43	5.72
9.80	0.320	0.105	9.20	6.50	3.124	1.56	-0.04	0.73	12.0	11.13	6.75	15.76	9.55
13.0	0.327	0.051	10.0	8.10	2.292	1.38	-0.01	1.15	5.67	13.87	8.41	17.90	10.8

Table 2: The Cyclic voltammetry parameters $[E_{Pc}, E_{Pa}, \Delta Ep, Ep_{c/2}, Da. Dc \alpha_{nc}, k_{sr}\Gamma_a, \Gamma_c, Q_a \text{ and } Q_c]$ of different scan rates 0.1 (mole.dm⁻³)HgCl₂in 0.05(mole.dm⁻³) NaClO₄ using glassy carbon electrode (GCE)

Scan rate Vs ⁻¹	E _{pa} (V)	(-)E _{pc} (V)	[-)I _{Pa} μΑ	Ι _{Ρc} μΑ	Dax10 ⁻¹⁰ Cm ² .s ⁻¹	Dcx10 ⁻¹¹ Cm ² .s ⁻¹	Ep _{c/2} V	αna	k _s x10 ⁻³ Cm ² .S ⁻¹	$\frac{\Gamma_c 10^{-9}}{mol/c}$ $\frac{m^2}{m^2}$	(+) Q _c x10 ⁻⁵ colomb	Γ _a x10 ⁻⁸ mol/cm ²	(-) Q _a x10 ⁻⁵ Colomb
0.1	0.332	0.526	146.00	62.60	2.25	0.041	-0.656	-0.3731	9.10	5.39	3.27	1.258	7.63
0.05	0.323	0.731	73.30	80.70	1.14	0.137	-0.494	0.204	9.25	13.91	8.43	1.264	7.66
0.02	0.292	0.759	74.20	91.80	2.91	0.452	-0.445	0.154	8.63	39.57	24.0	3.198	19.4
0.01	0.201	0.791	62.30	100.00	4.10	1.056	-0.370	0.115	2.62	86.22	52.2	5.371	32.2

Scan Speed effect

Figure 2 (a and b) represents effect of different scan rate on redox reaction of mercuric chloride.

The solvation and kinetic parameters of different scan rates of lead ions were presented in Table 2. All the solvation cyclic voltammetry data, given in

Table 2, are affected by different scan ratesindicating diffusibility of solvation.



Figure 2: Cyclic voltammetry of different scan rate 0.1 (mole.dm⁻³) HgCl₂ (drawn from origin program) with the original cyclic voltammograms at right side

Electro-behavior of mercuric ions in presence of (Diamond Fuchsin) at 303 K

Figure 3 and Tables 3 and 4 represent the different dye used on the solvation parameters for mercuric chloride in 0.05 M NaClO₄. From the previous figures, it was observed the formation of the complex appear in decreasing the anodic and cathodic peak beside the potential shifts to new

values. The electrochemical redox behavior of lead ions in the presence of a ligand such as diamond fuchsin at 303 K at the GCE was studied, and the steady-state current of the ions examined was obtained and explained using different equations. The solvation and kinetic parameters of the interaction of mercuric ions and different concentrations of diamond fuchsin at 303 K and a scan rate of 0.1 V/S were presented in Table 3 (a and b).



Figure 3: Cyclic voltammetry of HgCl₂in 0.05 (mole.dm⁻³) NaClO₄and diamond fuchsin (Diamanten)

[L] x10 ⁻⁴ M	E _{pa} (V)	(-)E _{pc} (V)	(-)I _{Pa} μΑ	I _{Pc} μΑ	D _a x10 ⁻ 11 cm ² .s ⁻¹	D _c x10 ⁻ 10 cm ² .s ⁻¹	(-) Ep _{c/2} V	αn _a	k _s x10 ⁻⁵ cm.s ⁻¹	$\Gamma_{c} ext{ x10^{-8}} \\ ext{mol/cm}^{2}$	Q _c x10 ⁻⁴ Coulomb	Γ _a x10 ⁻⁹ mol/cm ²	Q _a x10 ⁻⁵ Coulomb
1.62	0.331	0.957	69.80	103.00	10.31	2.25	0.246	0.067	7.32	1.76	1.07	11.95	7.25
3.23	0.335	0.998	25.30	149.00	1.36	4.73	0.513	0.099	30.00	2.55	1.55	4.33	2.63
4.82	0.337	1.012	22.10	813.00	1.05	14.20	0.722	0.165	0.28	13.92	8.44	3.78	2.29
7.99	0.355	1.923	10.50	954.00	0.23	19.80	0.761	0.041	2.12	16.34	9.90	1.79	1.09

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Table 3: The Cyclic voltammetry parameters of HgCl₂in 0.05 (mole.dm⁻³) NaClO₄and diamanten fuchsin



Figure 4: Cyclic voltammetry of different scan speed of HgCl₂ in 0.05 NaClO₄ (mole.dm⁻³) and Diamond Fuchsin.

Table 4: The Cyclic voltammetry parameters of different scan rates in 0.05 M NaClO₄ for M (HgCl₂) and ligand (L), diamenten fuchsin on using glassy carbon electrode (GCE)

scan rae V. s ⁻¹	E _{pa} (V)	(-)E _{pc} (V)	(-)I _{Pa} μΑ	I _{Pc} μΑ	D _a x10 ⁻ 12 cm ² .s ⁻¹	D _c x10 ⁻ 11 cm ² .s ⁻¹	(-) Ep _{c/2} V	αna	k _s x10 ⁻³ cm.s ⁻¹	Γ _c x10 ⁻⁹ mol/cm ²	Qc x10 ⁻⁵ Coulomb	Γa x10 ⁻⁹ mol/cm ²	Qa x10 ⁻⁶ Coulomb
0.1	0.346	0.96	98.20	92.80	1.150	10.02	0.477	0.099	0.116	7.948	4.82	0.841	5.10
0.05	0.373	0.837	75.80	41.20	1.370	4.05	0.465	0.129	0.925	7.057	4.28	1.298	7.87
0.02	0.332	0.75	16.50	26.80	0.162	4.284	0.359	0.109	4.98	11.48	6.95	0.706	4.28
0.01	0.313	0.734	16.00	18.10	0.305	3.908	0.203	0.090	1.47	15.503	9.39	1.370	8.30

Most of the solvation parameters especially the cathodic surface coverage Γ_c , the anodic surface coverage Γ_a , the cathodic quantity of electricity Q_c , and anodic quantity of electricity \mathbf{Q}_a are increased by enhanced the ligand concentration indicting more complexation reaction.

The thermodynamic parameters for the interaction of mercuric ions with ligand are evaluated and the resulted data are presented in Table 5 [30-35]. All the data given in the previous tables and figures prove that there is an interaction of the type electrostatic interaction

between the mercuric ions and diamond fuchsin and this reaction is controlled by diffusion mechanism reaction and fast reaction with small electron transfer rate constant. Furthermore, the addition of diamond fuchsin to mercuric ions gave smaller cyclic voltammetry data than mercuric ions alone proving the interaction is thoughts the complexation reaction. All data are decreased by increase scan rate supporting the diffusion mechanism. *Complexation between Diamond Fuchsin and Mercuric Chloride*

The complexation thermodynamics were evaluated as explained in previous paper from cyclic voltammetry data [19-30] and the evaluated data are listed in Table 5 proving the interaction by complexation between the two materials.

Table 5: The Value of (stability constant $\log \beta j$ and Gibbs free energy ΔG) for HgCl₂ +Diamenten complex at scan rate 0.1 V.s⁻¹

[M] x10 ⁻³ mole.dm ⁻³	[L] x10-4 mole.dm ⁻⁴	E _{PC} (L)	E _{PC} (C)	ΔE (V)	log[L]	log βj	ΔG (KJ/mol ⁻¹)
1.30	1.62	0.327	0.331	-0.004	-3.790	0.338	-1.948
1.28	3.23	0.327	0.335	-0.008	-3.491	0.612	-3.529
1.27	4.82	0.327	0.337	-0.01	-3.316	0.924	-5.333
1.25	7.99	0.327	0.355	-0.028	-3.097	1.042	-6.009

Scan speed effect Hg²⁺⁻- Diamond Fuchsin Complex

The effect of different scan rates on the interaction between mercuric and Diamond Fuchsin was studied in different scan speeds (0.1, 0.05, 0.02, and 0.01) V/S at 303 K. The solvation and kinetic parameters of different scan rates for the studied complex were presented in Tables 4 and 5.

Most of the solvation data provided in Table 5 show increase in their values by decrease of the scan rate favoring more diffusion mechanism. R²

values were estimated for some data and found to be in the range of 1.

Rosaniline (Dimond Fuchsin) docking with Estrogen Receptor alpha Code id (7Y8G) Breast cancer ($Er\alpha$)

The molecular docking was calculated from the interaction between the very effective Rosaniline (diamond fuchsin) with Estrogen Receptor alpha Code id (7Y8G) Breast cancer ($\text{Er}\alpha$) protein (Table 6, Figure 5).

Table 6: Interaction parameters between Rosaniline (Dimond Fuxhsin) docking with Estrogen Receptor alphaCode id alpha (7Y8G)

Rosaniline	Receptor	Interaction	Distance (A°)	E (kcal/mol)
N 31	OG1 THR 347 (A)	H-donor	3.02	-1.9
N 37	0E1 GLU 353 (A)	H-donor	3.02	-5.2
N 37	0E2 GLU 353 (A)	H-donor	3.49	-0.5
N 37	0 LEU 387 (A)	H-donor	3.33	-0.9
N 37	OE1 GLU 353 (A)	Ionic	3.02	-4.4
N 37	CE1 PHE 404 (A)	pi-H	3.49	-1.9
6-ring	CE1 PHE 404 (A)	pi-H	3.94	-0.7

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Figure 5: Rosaniline (dimond fuchsin) 2D and 3D pose docking with Estrogen Receptor alpha Code id (7Y8G) Breast cancer (Erα) modes of interaction

Dye docking, known as molecular docking is technique used to study the binding interactions between small molecules (ligand) and a target protein such as the estrogen receptor alpha ($Er\alpha$).

By predicting and alayzing the binding mode and affinity of a ligand with the receptor dye docking can provide valualble insights ubto the ligandreceptor interactions, which can futther utilizes for drug discovery and design. In the context of the estrogen receptor alpha ($Er\alpha$), it is a nuclear hormone receptor that plays a crucial rolein mediating the effects of estrogen in various tissues. (Er α) is a transcription factor that regulates the expression of target genes upon binding to esttrogen or estrgen-like compounds. Dye regulation of $(Er\alpha)$ signalising has been emplicated in several diseases, including breast cancer and osteoporosis.Once the docking simulation is complete, the software will rank the generated possess based on a scoring function that estimates the binding affinity. The predeicted binding mode and affinity can can provide insights into the ligands potential for binding to ($Er\alpha$) and modulating its activity.

It is important to note that dye docking is a computational technique and predicted results should be experimentally validated to confirm the accuracey and realiability of the predications.Experimental rechniques like X-ray and NMR spectroscopy can be employed to validate the binding interactions.

Conclusion

1- Increase of the solvation parameters for mercuric chloride by increase in its concentrations due to the diffusion and preconcentration reaction.

2- Sharp detection of reduction and oxidation peaks for mercuric ions alone and in presence of ligand.

3- Effect of different Diamond Fuchsin concentrations on adding to mercuric chloride were studied cyclic voltammetrically and found to decrease in most solvation parameters by increasing ligand concentrations indicating interaction between them.

4- Effect of different scan speeds on interaction between mercuric chloride and Diamond Fuchsin are studied and found to decrease by increase in scan speeds indicating reversibility of the waves.

5- The stability constants and Gibbs free energies of complexation are calculated and found to be electrostatic interaction.

Increase the area of the used materials for the metal in presence of ligand used under the cyclic

voltammograms, indicate the increase of storage capacity which facilitate its uses in energy storage.

Highlights

1- Estimation of the cyclic voltammetry data for redox reaction of mercuric chloride alone and in presence of ligand Diamond Fuchsin.

2- Study the different scan speeds for mercuric chloride in 0.05 M NaClO₄ alone and in presence of Diamond Fuchsin.

3- Estimation of the stability constants and Gibbs free energies of complexation for (1:1) complexes for metal to ligand.

4- Estimate docking parameters for interaction of Roseaniline with estrogen receptor alpha Code id (7Y8G) breast cancer ($\text{Er}\alpha$) protein.

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Authors' contributions

All authors contributed toward data analysis, drafting, and revising the paper and agreed to responsible for all the aspects of this work.

Conflict of interest

The authors declare that they have no conflicts of interest in this article.

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