Solvation Data for the Redox Interaction Between Nano Cobalt Sulfate (NCS) and Fuchsin Acid (FA) Using Doped Nano Composite+ Multicarbon Nanotubes Glassy Carbon Electrode at Different Temperatures

Esam A Gomaa (✉ aa.sh_04@yahoo.com)

Faculty of Science <https://orcid.org/0000-0002-9686-4860>

H A Killa

Faculty of Science

H Fathi

Faculty of Science

A Farouk

Faculty of Science

Research Article

Keywords: Fuchsin acid, Nano cobalt sulphate salt, Doped nano glassy carbon electrode, Cyclic voltammetry, Thermodynamic parameters, 5C5S, Molecular docking

Posted Date: December 22nd, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-1159797/v1>

License: This work is licensed under a Creative Commons Attribution 4.0 International License. [Read Full License](#)

Abstract

Preparation of nano tantalum pentoxide and nano cobalt sulfate were prepared by ball milling using Retsch MM2000 apparatus with three stainless steel balls having diameter 12 mm. Preparation of new working electrode was done by adding nano tantalum pentoxide to multicarbon nanotubes and carbon with specific ratio and finish nano paste put at the tip of glassy carbon electrode and used for use.

The redox reaction of nano cobalt sulfate were studied in 0.1M KBr alone at two temperatures 292.15K and 297.15 using cyclic voltammetry. Different solvation and kinetic parameters were calculated at the used two temperatures and their data were discussed. Interaction parameters of the nano cobalt sulfate with Fuchsin acid dye was done to study the complexation character between the two cyclic voltammetrically and the resulted data are discussed. Different thermodynamic data were evaluated for the interaction of nanocobalt sulfate NCS with Fuchsin Acid, FA like stability constants, Gibbs free energies of complexation, enthalpies and entropies were evaluated and their values were discussed

1. Introduction

Progress in the study of magnetic nanoparticles have been made because of their properties and potential uses [1]. The potential applications of magnetic nanoparticles as cobalt sulfate in field of data storage, medical diagnosis and catalytic magnetic and electrical properties have been achieved [2-4]. Cobalt sulfate received more attention in last years due to its catalytic, electrical and medicinal applications. Cobalt sulfate is one of the most ferromagnetic materials due to its three metastable phases with different crystallographic structures [5,6].

Cobalt sulfate is used electroplating and electrochemical industries [5]. It added to nickel plating to improve the smoothness, brightness, hardness and ductility of the deposited materials. It used as drier for lithographic inks, varishes, paints and in storage batteries. Cobalt sulfate was used to improve hematocrit, hemoglobin and erythrocyte levels in human patients with refractory anemia, including sickle-cell disease, thalassemia, chronic renal disease [6]

2. Experimental

2.1. Materials and Solvents

The chemicals used in the present study were pure cobalt sulfate salt (CoSO_4) from Merck Company, fuchsin acid (FA) from Oxford Laboratory, pure potassium bromide salt (KBr) from Adwic Company and bidistilled water prepared with conductivity of $3.2 \mu\text{S cm}^{-1}$.

Also, the chemicals used for preparation of doped nano glassy carbon electrode were pure tantalum pentoxide salt (Ta_2O_5) from BDH Middle East FZ LLC, Graphite powder from Adwic Egypt and carbon nano-tube from Egyptian Petroleum Research Institute.

Fuchsin acid (FA)	
Disodium 2-amino-5-[(Z)-(4-amino-3-sulfonatophenyl)(4-iminio-3-sulfonato-2,5-cyclohexadien-1-ylidene)methyl]-3-methylbenzenesulfonate	
Formula	$C_{20}H_{17}N_3Na_2O_9S_3$
Mol. wt.	585.53 g·mol ⁻¹

2.2. Preparation of nano salts .

Nano cobalt sulphate (NCS) was prepared by shacking bulk cobalt sulphate salt($CoSO_4$)in ball-mill apparatus of type Retsch MM2000 swing mill for two hours. The ball milling was performed at 20225 Hz and at room temperature using stainless steel tubes with volume equal 10 cm³ and three stainless steel balls with diameter of 12 mm. Also, nanotantalumpentoxide salt was prepared by the same ball milling method from bulk tantalum pentoxide salt (Ta_2O_5).Finally, the resulting nanoparticles were investigated under transmission electron microscope (TEM).

2.3. Preparation of doped nano composite glassy carbon electrode.

Nanocomposite carbon paste was prepared by mixing [80% graphite powder,10% paraffin wax, 5% nano tantalumpentoxide and 5% multi layers carbon nano tubes] very well to produce a homogeneous paste.Then the resulted paste was packed into the end of an electrode (depth:6mm). External electrical contact was established by forcing a copper wire down the electrode. The surface of the electrode was polished with a piece of weighting paper and then rinsed with distilled water thoroughly at room temperature. The resulting nanocarbon paste was investigated under transmission electron microscope (TEM).

2.4. Cyclic voltammetricanalysis (CV)

The cyclic voltammetric studies were done by using DY2000 multichannel potentiometer, delivered from USA. It was connected to a cell of three electrodes, silver/silver chloride put in saturated KBr solution used as reference electrode, doped nano compositeglassy carbon electrode (DGC) as working electrode and platinum wire as auxiliary electrode. The doped nano composite glassy carbon electrode (DGC) surface was polished to mirror state using 1-0,03 micro alumina powder and washed with absolute alcohol and doubly-distilled water till removing any adhering alumina particles. Area of electrode was (5.72×10^{-2}) cm². The system was applied from (0.4 to -1.5)V potential window and different scan rates (0.1, 0.05, 0.02, 0.01)V/sec at two different temperatures (292.15 and 297.15)K. Passing purified N₂ was done before each experiment to insure inert atmosphere and diffusion experiment. Finally, the data was analyzed using origin software.

2.5. Molecular Docking

The Molecular Operating Environment (MOE) was used as molecular modeling to rationalize the observed anticancer activity of fuchsin acid (FA) with the crystal structure of human Myosin 9b RhoGAP domain at 2.2 Angstrom (5C5S).

The molecular modeling and computational calculations were carried out by using DS Biovia material studio 2017, software material studio 07.0, Gaussian 09 and Docking Server software.

3. Results And Discussion

3.1.Transmission electron microscopy (TEM)

Transmission electron microscope was used to discover the internal structure and size of nanotantalumpentoxide, multi nano carbon nano tube paste of the used electrode and nano Nano cobalt sulphate salt, **Fig. 1**.

It was found that nanocobalt sulfate is in the form of distorted hexagonal forms in size range from 19 nm to 27 nm.Nano tantalum pentoxide is in the form of irregular spheres with size in the range between 60-72 nm.

3.2.Cyclic voltammetry (CV)

3.2.1. Electrochemical behavior of nano cobalt sulphate salt (NCS)alone at two different temperatures.

3.2.1.1. Effect of different nanocobaltsulphate salt (NCS) alone at 292.15 and 297.15K.

The cyclic voltammogram of a supporting electrolyte KBr (0.1) M was measured from (0.4 to -1.4) V using doped nano glassy Carbon electrode (DGC) by DY2000 multichannel potentiometer at 292.15 and 297.15K, Fig. 2. Then, the redox behavior of nano-Co²⁺ was examined in 0.1 M KBr by adding nano-Co²⁺ ions solution step wisely from 1 ml (1.77 x10⁻³) M to 6 ml (9.17 x10⁻³) M at 292.15 and 297.15K, Fig. 3.

The appearance of reduction wave at -0.5 V and oxidation at 0.4 may due to oxygen wave in supporting electrolyte which disappears on adding cobalt solution.

The electrochemical redox behavior of nanoCo²⁺ ions alone in KBr (0.1) M was studied at the steady state current, cyclic waves were obtained and explained using the following equations [5–23].

$$i_p = 0.4463 n F A C (n F D v / R T)^{1/2} \quad \text{Randles-Sevcik equation (1)}$$

$$\Delta E_p = E_{pa} - E_{pc} \quad (2)$$

$$k_s = 2.18 [D_c \alpha n_a F v / RT]^{1/2} \exp [\alpha^2 n F \Delta E_p / RT] \quad (3)$$

$$\alpha n_a = 1.857 RT / (E_{pc} - E_{pc/2}) F \quad (4)$$

$$\Gamma = i_p 4RT / n^2 F^2 A v \quad (5)$$

$$Q = n F A \Gamma \quad (6)$$

Where, i_p is the current in Ampere, A is the surface area of working electrode in cm², D is the diffusion coefficient in cm²/Sec, v is the scan rate in volts/Sec and C is the Bi³⁺ concentration, ΔE_p is the peak potential difference, k_s is the standard heterogeneous electron transfer rate constant in cm/sec, α is charge transfer coefficient and n_a is the numbers of electron transfer in the rate determining step, $E_{pc/2}$ is the half wave potential for cathodic peak, Γ is the surface coverage in mol.cm⁻² and the quantity of charge consumed during the reduction or adsorption of the adsorbed layer Q can be used to calculate the surface coverage.

The calculated solvation and kinetic parameters are E_{pa} (anodic peak potential), E_{pc} (cathodic peak potential), i_{pa} (anodic peak current), i_{pc} (cathodic peak current), ΔE_p (peak potential difference), D_a (anodic diffusion coefficient), D_c (cathodic diffusion coefficient), k_s (electron transfer rate constant), Γ_a (anodic surface coverage), Γ_c (cathodic surface coverage), Q_a (anodic quantity of electricity) and Q_c (cathodic quantity of electricity) are tabulated in Table.1 (a,b).

On reduction wave was observed in the window range used from 0.4V to -1.4V at the experimental two used temperatures which are 292.15 and 297.15K. The oxidation proceed through two waves as shown in Figs. 1 and 2. We noticed that same trend was followed at the two temperatures with more defined waves at the higher temperature,

Table.1(a)

The solvation and kinetic parameters of different NCS concentrations at 292.15 K and scan rate 0.1 V/sec.

[M] x 10 ⁻³	Ep,a	Ep,c	ΔEp	ΔEp (mV)	(-)Ip,a x 10 ⁻⁵	Ip,c x 10 ⁻⁴	Da x 10 ⁻¹³	Dc x 10 ⁻¹¹	ks	Γ a x 10 ⁻⁹	Γ c x 10 ⁻⁸	(-) Q a x 10 ⁻⁵	(+) Qc x 10 ⁻⁴
1.774	0.3195	0.9461	0.6266	626.61	1.62	1.17	4.403	2.315	6.553	0.739	0.535	0.8157	0.591
3.438	0.3195	0.9390	0.6195	619.48	2.59	1.63	2.989	1.191	4.101	1.180	0.744	1.302	0.821
5.000	0.2740	0.9490	0.6750	675.00	4.49	2.36	4.256	1.179	10.17	2.048	1.078	2.260	1.189
6.471	0.2721	0.9555	0.6834	683.36	6.28	3.08	4.973	1.200	10.99	2.865	1.407	3.162	1.553
7.857	0.2721	0.9651	0.6930	692.98	6.67	3.28	3.801	0.918	10.64	3.041	1.495	3.356	1.650
9.167	0.2740	0.9746	0.7006	700.59	7.15	4.42	3.212	1.225E-11	15.38	3.261	2.014	3.600	2.223

Table.1(b)

The solvation and kinetic parameters of different NCS concentrations at 297.15 K and scan rate 0.1 V/sec.

[M]x10 ⁻³	Ep,a	Ep,c	ΔEp	(-)Ip,a x10 ⁻⁵	Ip,c x10 ⁻⁴	Da x10 ⁻¹³	Dc x10 ⁻¹²	ks	Γ c x10 ⁻⁸	(+) Qc x10 ⁻⁴	Γ a x10 ⁻⁹	(-) Q a x10 ⁻⁵
1.77	0.4198	1.0242	0.6043	0.5033	0.2612	0.4249	1.144	0.583	0.121	0.133	0.2335	0.2577
3.44	0.3413	0.9760	0.6346	2.780	1.373	3.452	8.428	2.587	0.637	0.7033	1.290	1.423
5.00	0.3149	0.9254	0.6105	4.713	2.541	4.691	1.363	2.650	1.179	1.301	2.187	2.413
6.47	0.3043	0.9289	0.6245	5.903	2.749	4.393	9.527	2.679	1.275	1.408	2.738	3.023
7.86	0.2779	0.9462	0.6683	7.241	3.072	4.484	8.071	4.958	1.425	1.573	3.359	3.708
9.17	0.2169	0.9936	0.7766	12.73	4.746	10.18	14.15	46.493	2.202	2.430	5.907	6.520

We observe the following from Table 1a and 1b:

1-Epc and Epa are increased at higher temperature than that at lower one.

2-Ipa and Ipc are bigger at 297.15K than that at 292.15K.

3-Da and Dc are increase by at high temperature than that at lower one.

4-ks is very high at 297.15K using 9.17x10⁻⁴M Fuchsin acid FA than others.

5- Γ a and Γ c are decreased at temperature 297.15K than that at 292.25K due to the migration of products away from the surface of electrode by more increase of temperature.

6- Qa and Qc are decreased at 297.15K than 292.15K due to migration of ions.

3.2.1.2. Effect of different scan rates

The cyclic voltammogram of NCS (9.17x10⁻³) M in KBr (0.1) M was studied at different scan rates (0.1, 0.05, 0.02 and 0.01)(V/sec) and two different temperatures (292.15 and 297.15)K, **Fig. 4**. Then the solvation and kinetic parameters at the different scan rates can be calculated, **Table.2(a,b)**.

The appearance of maxima in Fig. 4 are mainly due to adsorption, catalysis and electro catalysis of the adsorbed species to the nano electrode surface. This maxima appeared only by the use of multicarbon nano tube electrode due to the great adsorption at the working electrode for the ionic species by using multi polymer nano electrode. The competition between adsorption and dehydration also explains the voltammetric behavior. In order to observe the catalytic mechanism, minimum coverage is necessary as shown for Γ_a and Γ_c in Tables 2a and 2b.

Table.2 (a)

The solvation and kinetic parameters of (9.17×10^{-3}) MNCS at different scan rates and 292.15 K.

ν	E_{p_a}	E_{p_c}	ΔE_p	$(-)I_{p_a}$ $\times 10^{-5}$	I_{p_c} $\times 10^{-4}$	D_a $\times 10^{-13}$	D_c $\times 10^{-12}$	k_s	Γ_a $\times 10^{-9}$	Γ_c $\times 10^{-8}$	$(-)Q_a$ $\times 10^{-5}$	$(+)Q_c$ $\times 10^{-4}$
0.1	0.2740	0.9746	0.7006	7.150	4.415	3.212	12.25	15.38	3.261	2.014	3.600	2.223
0.05	0.2781	0.9453	0.6672	5.060	3.241	3.218	13.20	6.262	4.616	2.956	5.095	3.263
0.02	0.3125	0.8861	0.5736	2.465	1.617	1.910	8.214	0.516	5.623	3.688	6.206	4.071
0.01	0.3240	0.8321	0.5081	1.586	0.970	1.581	5.918	0.112	7.235	4.427	7.986	4.886

Table.2 (b): The solvation and kinetic parameters of (9.17×10^{-3}) MNCS at different scan rates and 297.15 K.

ν	E_{p_a}	E_{p_c}	ΔE_p	$(-)I_{p_a}$ $\times 10^{-5}$	I_{p_c} $\times 10^{-4}$	D_a $\times 10^{-13}$	D_c $\times 10^{-12}$	k_s	Γ_a $\times 10^{-9}$	Γ_c $\times 10^{-8}$	$(-)Q_a$ $\times 10^{-5}$	$(+)Q_c$ $\times 10^{-4}$
0.1	0.2169	0.9936	0.7766	12.73	4.746	10.18	14.15	46.493	5.907	2.202	6.520	2.430
0.05	0.2933	0.9453	0.6520	6.838	2.808	5.876	9.907	2.511	6.345	2.605	7.003	2.876
0.02	0.3332	0.8861	0.5529	3.646	1.523	4.177	7.289	0.234	8.458	3.533	9.336	3.900
0.01	0.3502	0.8321	0.4819	2.468	0.892	3.829	5.005	0.051	11.45	4.141	12.64	4.570

Effect of scan rates show increase in most of the solvation parameters at higher temperature in Tables 2a and 2b indicating more solvation.

The relation between cathodic and anodic peak current against the square root of scan rate was applied using Randles-Sevcik equation [24–28] which gives straight lines to indicate the diffusion process, Fig. 5.

3.2.2. Electrochemical behavior of nanocobalt sulphate salt (NCS) in presence of Fuchsin acid (FA) at two different temperatures.

3.2.2.1. Effect of different Fuchsin acid (FA) at 292.15 and 297.15 K.

The electrochemical behavior of the complexation between NCS and FA was studied in 0.1M KBr and scan rate 0.1 V/sec at 292.15 and 297.15 K, Fig. 6. The solvation and kinetic parameters of interaction of NCS (9.17×10^{-3}) M and different concentrations of FA at 292.15 and 297.15 K and scan rate 0.1 V/sec were presented in Table.3 (a,b).

Fuchsin acid increases the maxima appeared for Co^{+2} ions in 0.1M KBr solution. In the reduction window due to the increase in the dehydration and catalysis of the adsorbed ions. This proves that the use of Fuchsin acid increases the adsorbed ions and the ionization of the used aqueous solutions.

Table.3(a)

Effect of different concentrations of FA for redox peak at 292.15 K.

[M] x10 ⁻³	[L] x10 ⁻⁴	Ep,a	Ep,c	ΔEp	(-)Ip,a x10 ⁻⁵	Ip,c x10 ⁻⁴	Da x10 ⁻¹⁴	Dc x10 ⁻¹³	ks	(-) Q _a x10 ⁻⁵	(+) Q _c x10 ⁻⁴	Γ a x10 ⁻⁹	Γ c x10 ⁻⁹
8.919	2.70	0.2642	0.9863	0.7222	4.79	2.88	15.21	55.22	14.099	2.410	1.452	2.184	13.16
8.684	5.26	0.2845	0.9826	0.6981	4.00	2.15	11.19	32.44	6.731	2.013	1.084	1.823	9.81
8.354	8.86	0.3539	0.9566	0.6028	3.36	1.51	8.555	17.16	0.880	1.693	0.758	1.534	6.869
8.250	10.0	0.3683	0.9542	0.5859	3.14	1.10	7.667	9.431	0.543	1.583	0.555	1.434	5.030
8.049	12.2	0.3723	0.9560	0.5836	2.99	0.981	7.303	7.846	0.463	1.507	0.494	1.365	4.475
7.857	14.3	0.3817	0.9595	0.5778	2.86	0.878	7.017	6.598	0.378	1.442	0.442	1.307	4.006

Table.3(b)

Effect of different concentrations of FA for redox peak at 297.15K.

[M] x10 ⁻³	[L] x10 ⁻⁴	Ep,a	Ep,c	ΔEp	(-)Ip,a x10 ⁻⁵	Ip,c x10 ⁻⁴	Da x10 ⁻¹⁴	Dc x10 ⁻¹²	Ks	Γ a x10 ⁻⁹	Γ c x10 ⁻⁸	(-) Q _a x10 ⁻⁵	(+) Q _c x10 ⁻⁴
8.92	2.70	0.2542	0.9735	0.7193	9.858	4.968	64.51	16.38	17.151	4.574	2.305	5.048	2.544
8.68	5.26	0.2560	0.9711	0.7151	9.013	4.579	56.87	14.68	14.924	4.181	2.124	4.615	2.345
8.35	8.86	0.2656	0.9581	0.6925	5.281	3.762	21.09	10.71	8.890	2.450	1.745	2.704	1.927
8.25	10.0	0.2927	0.9571	0.6644	2.570	3.241	5.123	8.147	4.709	1.192	1.504	1.316	1.660
8.05	12.2	0.3863	0.9336	0.5473	1.311	2.474	1.400	4.987	0.422	0.608	1.148	0.671	1.267
7.86	14.3	0.3863	0.9291	0.5428	1.195	1.875	1.221	3.007	0.350	0.554	0.870	0.611	0.960

We noticed decrease in most of the solvation parameters for nano cobalt sulfate NCS by adding Fuchsin acid FA and is decreased on usat 297.15 K than 292.15K indicating complexationcharater.Also the surface coverage parameters for Co²⁺ ions are decreased on adding Fuchsin acid in 0.1 M KBr facilitating the happened of linear cathodic maxima. The maxima are decreased by the decrease in the scan rate.

3.2.2.2. Effect of different scan rates

Effect of different scan rates on the interaction between NCS and FA was studied at different scan rates (0. 1, 0.05, 0.02 and 0.01) (V/sec), **Fig. 7**.Then the solvation and kinetic parameters at the different scan rates can be calculated,**Table.4(a,b)**.

Also, the relation between cathodic and anodic peak current I_pagainst the square root of scan rate in 0.1M KBr were shown in **Fig. 8**.

Table.4(a)

Effect of different scan rate of complex for redox peak at 292.15K.

□	Ep _a	Ep _c	ΔE _p	(-)Ip _a x10 ⁻⁵	Ip _c x10 ⁻⁵	Da x10 ⁻¹⁵	Dc x10 ⁻¹³	k _s	Γ _a x10 ⁻⁹	Γ _c x10 ⁻⁹	(-)Q _a x10 ⁻⁵	(+)Q _c x10 ⁻⁵
0.1	0.3817	0.9595	0.5778	2.864	8.783	7.017	6.598	0.3776	1.307	4.006	1.442	4.422
0.05	0.4218	0.9486	0.5269	1.469	6.084	3.693	6.330	0.0858	1.340	5.550	1.480	6.126
0.02	0.4642	0.9225	0.4583	0.598	3.631	1.530	5.639	0.0143	1.364	8.282	1.506	9.142
0.01	0.4742	0.9003	0.4261	0.257	1.818	0.565	2.825	0.0050	1.173	8.290	1.295	9.151

Table.4(b)

ν	E_{pa}	E_{pc}	ΔE_p	$(-)I_{pa}$	I_{pc}	D_a	D_c	k_s	Γ_a	Γ_c	$(-)Q_a$	$(+)Q_c$
				$\times 10^{-5}$	$\times 10^{-4}$	$\times 10^{-16}$	$\times 10^{-12}$		$\times 10^{-10}$	$\times 10^{-8}$	$\times 10^{-6}$	$\times 10^{-4}$
0.1	0.3863	0.9291	0.5428	1.195	1.875	122.1	3.007	0.350	5.543	0.8700	6.119	0.9603
0.05	0.4738	0.9067	0.4329	0.331	1.094	18.80	2.046	0.028	3.076	1.015	3.395	1.120
0.02	0.5040	0.8838	0.3798	0.0809	0.682	2.805	1.992	0.008	1.879	1.583	2.074	1.747
0.01	0.5039	0.8756	0.3717	0.0400	0.414	1.368	1.469	0.004	1.856	1.923	2.048	2.123

Effect of scan rate for NCS+FA was observed in Tables 4a and 4b, showing decrease in all values at 297.15K than that at 292.15K due also to the complexation character.

3.2.3. Electrochemical behavior of the complexation between NCS and FA.

The stability constants (β_{MX}) for $Bi(NO_3)_3$ complexes for each addition are calculated by applying the following equations [24–27]:

$$\Delta E^\circ = E^\circ_C - E^\circ_M = 2.303 (RT/nF) * (\log \beta_{MX} + j \log C_x) \quad (7)$$

$$E^\circ = (E_{pa} + E_{pc})/2 \quad (8)$$

$$\Delta G = -2.303 RT \log \beta_{MX} \quad (9)$$

Where E°_M is the formal peak potential of metal at finally adding in the absence of FA, E°_C is the formal peak potential of metal complex after each addition of FA, R is a gas constant ($8.314 \text{ J.mol}^{-1}.\text{degree}^{-1}$), T is the absolute temperature, j is the coordination number of the stoichiometric complex and C_x is the concentration of FA in the solution. E_{pa} and E_{pc} are anodic peak potential and cathodic peak potential, respectively and the Gibbs free energy of interaction ΔG for NCS with FA were calculated from stability constant (β_{MX}).

The relation between Gibbs free energy against stability constant of $Bi(NO_3)_3$ complexes with CFZ were shown in **Fig. 9**.

By using Van't Hoff equation (10), the enthalpy (ΔH) of interaction for NCS with FA was calculated.

$$\log \frac{\beta_{MX} \text{ at } (T_2)}{\beta_{MX} \text{ at } (T_1)} = \frac{\Delta H}{2.303} \left(\frac{T_2 T_1}{T_2 - T_1} \right)$$

10

where β_{MX} is the stability constant at different temperature, both T_2 and T_1 are 292.15 K and 297.15 K, respectively.

Also, the entropy (ΔS) for the formed complex between NCS and FA at the used two different temperatures were calculated by using Eq. (11)

$$\Delta S = \frac{\Delta H - \Delta G}{T}$$

11

The calculated values of β_{MX} , ΔG , ΔH , and ΔS for the formed complex were collected in **Table.5**.

Table.5

The stability constant β_{MX} , Gibbs free energy ΔG , enthalpy ΔH and entropy of interaction ΔS for the formed complex at 292.15 and 297.15K.

[M] x10 ⁻³	[L] x10 ⁻⁴	j	log β _j		ΔG (KJ/mol)		ΔH (KJ/mol)	ΔS (KJ/mol)
			292.15K	297.15	292.15K	297.15		
9.041	1.370	0.0152	0.2310	0.4979	-1.2921	-2.8327	716.58	2.457
8.919	2.703	0.0303	0.1429	0.4001	-0.7994	-2.2763	930.64	3.188
8.800	4.000	0.0455	0.3776	0.4407	-2.1120	-2.5076	388.07	1.336
8.684	5.263	0.0606	0.5187	0.4813	-2.9017	-2.7385	296.07	1.023
8.571	6.494	0.0758	0.9448	0.6206	-5.2849	-3.5312	218.39	0.766
8.354	8.861	0.1061	1.3928	0.5484	-7.7909	-3.1200	130.89	0.475
8.250	10.00	0.1212	1.6407	1.0297	-9.1779	-5.8586	208.64	0.746
8.148	11.11	0.1364	1.7029	2.2960	-9.5258	-13.0631	448.22	1.567
8.049	12.20	0.1515	1.8177	2.2964	-10.1677	-13.0653	419.99	1.472
7.952	13.25	0.1667	1.9089	2.2582	-10.6778	-12.8482	393.28	1.383
7.857	14.29	0.1818	2.1147	2.2959	-11.8291	-13.0626	360.93	1.276

It was observed that all entropies are positive, all free energies are negative indicating spontaneous reactions. Whereas enthalpies are positive indicating endothermic reactions. The Gibbs free energies of interaction are increased by increase of ligand, dye concentration indicating more interaction.

3.3. Molecular docking

A molecular modeling study using the Molecular Operating Environment

(MOE) was performed to rationalize the observed anticancer activity of FA. The binding modes between FA and active sites of the crystal structure of human Myosin 9b RhoGAP domain at 2.2 angstrom (5C5S) was predicted using MOE, **Fig. 10**. The docking study of the inhibitor was performed with rmsd value (2.086 Å) and binding free energies of (-5.8502 kcal.mol⁻¹). Docking of FA with (5C5S) active sites revealed the presence of H-donor interactions between N atoms in FA and Asp288, Asn 279 amino acids residue as shown in **Fig. 11** and also, the interaction between O atoms in FA and Arg 212, Ala 205 amino acids residue. The molecular surface structure of FA with (5C5S) receptor was shown in **Fig. 12**.

References

1. S.H.Sun, Adv.Mater., 18(2006)393.
2. C.B.Murray, C.R.Kagan, M.G.Bawendi, Science, 270(1995)1335>
3. A.P.Alivisatos, Science, 27(1996)933.
4. A.H.Lu, E.L.Salabas, F.Schuth, Angew.Chem., Int.Ed., 46(2007)1222.
5. D.P.Dinepa, M.G.Bawendi, Angew.Chem.Int.Ed., 38(1999)1788.
6. Q.A.Pankhurst, J.Connolly, S.K.Jones and J.Dobson, J.Phy.D.Appl.Phys., 36(2003)0167.
7. E. Muller, Z. Electrochem. , 13, 133 (1907).
8. S.T. Mayer, and R.H. Muller, J. Electrochem. Soc., 139, 426 (1992).
9. M.N. AbdEL-Hady, Esam A. Gomaa, Anwer G. Al-Harazie, Journal of Molecular Liquids, 276 (2019) 970-985.
10. M.N. Abd El-Hady, E. A. Gomaa, R.R. Zaky, A.I. Gomaa, Journal of Molecular Liquids, 305 (2000) 112794.
11. Elsayed M. AbouElleel, Esam A. Gomaa and Mai S. Mashally, J. Biochem. Tech., 9 (2) (2018) 42-47.
12. Esam A. Gomaa, Moged A. Berghot, Mohamed R. Moustafa, Fathy M. Eltaweel, Hadeer M. Farid, J. Marterials and Environmental Sciences, 10 (2019) 187-194.
13. Laila I. Ali, Shima A. Abdel Halim, Esam A. Gomaa, Sameh G. Sanad, Iran. J. Chem. Eng., 38 (2019) 43-58.
14. Esam A. Gomaa, Rania R. Zaki, Mai S. Nouh, Advanced J. of Chemistry Section A., 3, 5, (2020) 1-18.

15. F.A.Cotton, G. Wilkinson,"Advanced Inorganic Chemistry",4thEdn.,John Willey & Sons,New York, 1980.
16. P.L. Timmanagoounder, G.A.A. Hiremath, S.T. Nandibewoor, Trans. Met.Chem.,1997,22,193-196.
17. Y. Wang, R.M. Hernandez, D.J. Bartlett, J.M. Bingham, T.R. Kline, A. Sen& T.E. Mallouk, Langmuir ; 2006; 22(25), 10451-10456.
18. A.E. El-Askalany& A.M. Abou El-Magd, Chemical and Pharmaceutial Bulletin, 1995, 43, (10) , 1791-1792.
19. E.A. Gomaa, R.M. Abu-Qarn, Journal of Molecular Liquids,2017, 232, 319-324.
20. E.A. Gomaa, M.A. Tahooun, A. Negm, Journal of Molecular Liquids,2017, 241, 595-602.
21. E.A. Gomaa, R.R. Zaky, A. Shokr, Journal of Molecular Liquids,2017,232, 319-324.
22. E.A. Gomaa, R.R. Zaky, A. Shokr, Chemical Data Collections,2017, 11, 67-76.
23. E.A. Gomaa, A. Negm, M.A. Tahooun, Journal of Taibah University for Science, 2017, 11(5), 741-748.
24. S.E. El-Shereafy, E.A. Gomaa, A.M. Yousif, A.S. El-Yazed, Iranian Journal of Materials Science & Engineering, 2017, 14(4); 48-57.
25. J.I. Kim, A. Cecal, H.J. Born, E.A. Gomaa, Z. Phys. Chem., NeueFlog, 1978, 110-209.
26. J.I. Kim, E.A. Gomaa; Bull. Soc. Chim. Belg, 1981, 90 391.
27. M.A. Ghandour, R.A. Abo-Doma, E.A. Gomaa, Electrochim. Acta, 1982, 27, 159.
28. E.A. Gomaa, Thermochim. Acta, 1984, 80; 355.
29. A.K.Abd-Elkader, E.A. Gomaa, A.H. El-Askalany, 1985; ActaChimica Hung., 1985, 118; 197.
30. R.S. Nicholson, L. Shain, Analytical Chemistry, 1965, 37(2), 178-190.
31. G.A. Mabbotti, Journal of Chemical Education, 1983, 60(9), 697-702.
32. D.A.C. Brownson, C.E. Banks, The Handbook of Graphene Electrochemistry.; 2014; Springer.
33. E.A. Gomaa, M.A. Tahooun, M.A Journal of Molecular Liquids; 2016; 214, 19-23.
34. J.Wang, Analytical Electrochemistry-3rd ed., Jhon Wiley & Sons,, Inc.; London, 2006.
35. E.A. Gomaa, M.A.Tahooun, A.Shokr; Chemical Data Collections, 2016, 3-4, 58-67.
36. E.A. Gomaa, M.H. Mahmoud, M.G. Mousa, E.M. El-Dahshan, Chemical Methodologies, 2018, 3, 1-11.
37. E.A. Gomaa, G. Begheit, Asian J. of Chem., 2(1990) 444.
38. E.A. Gomaa, Monatshefte fur Chemie, 119(1988) 287.
39. M.A. Ghandour, E.A. Gomaa and R.A. Abo Doma, Monatisheftr fur Chemie, 116 (1985).
40. E.A. Gomaa, Radwa T. Rashed, Biomedical Journal of Scientific & technical Research, 2019, 23, 2, 17345-17349.
41. Casey P.Kelly, Christopher J.Cramer, Donald G. Truhlar, J. Phys. Chem., B., 2006, 110, 16066-16081.

Figures

Figure 1

TEM of (a) nanotantalumpentoxide salt (b) nano multi carbon nano paste (c) nanocobalt sulphate salt

Figure 2

Cyclic voltammogram of 30 ml KBr (0.1) M and scan rate 0.1 V/sec at 292.15 and 297.15K.

Figure 3

Effect of different NCS concentrations at (a) 292.15K (b) 297.15K and scan rate 0.1 V/sec.

Figure 4

Effect of different scan rates of (9.17×10^{-3}) M NCS at (a) 292.15 K (b) 297.15 K.

Figure 5

The relation between peak current I_p ($I_{p_c} - I_{p_a}$) against the square root of different scan rates at (a) 292.15K (b) 297.15K.

Figure 6

Effect of different concentrations of FA at (a) 292.15K (b) 297.15K and scan rate 0.1 V/sec.

Figure 7

Effect of different scan rates of (7.86 $\times 10^{-3}$) M FA with (14.3 $\times 10^{-4}$) M NCS at (a) 292.15 K (b) 297.15 K.

Figure 8

The relation between peak current I_p ($I_{pC} - I_{pA}$) against the square root of different scan rates in presence of FA at (a) 292.15 K (b) 297.15 K.

Figure 9

The relation between Gibbs free energy and Stability constant for the formed Complex at (a) 292.15K (b) 297.15K.

Figure 10

The binding mode of FA with (5C5S) receptor

Figure 11

The interaction between FA and (5C5S) receptor

Figure 12

The molecular surface structure of FA with (5C5S) receptor