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Theoretical model for spectroscopic study of Cu^{+2}, Co^{+2}, and Fe^{+3} dissolved in ethanol with a different concentrations

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Abstract

The absorption spectrum for three types of metal ions in different concentrations has been studying experimentally and theoretically. The examination model is Gaius model to find the best fitting curve and the equation controlled with this behavior. The three metal ions are (Copper chloride $CuCl_3$, Iron chloride Fe_2Cl_3, and Cobalt chloride $CoCl_3$) with different concentrations (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3. The spectroscopic study included UV-Visible and fluorescence spectrum for all different concentrations sample. The results refer to several peaks that appear from the absorption spectrum in the high concentration of all metal ions solution. The multiple absorption peaks continued even at the lowest concentration in the iron ion solution. Fluorescence spectrum shows intensive stimulating of the radiation strength was perceived in the manifestation of Cu^{+2}, Co^{+2} and Fe^{+3}. From modeling investigation, there are converge between experimental and theoretical results of the fluorescence spectrum for metal ions. Furthermore, identity and convergence which defined as (r^2), are on average (0.995).

Key words
Metal ions, spectroscopic study, Gaius model, UV-visible, fluorescence spectrum.

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انموذج نظري للدراسة الطيفية لـ Cu^{+2} و Co^{+2} و Fe^{+3} المذابة في الإيثانول بتراكيز مختلفة

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الخلاصة

تم دراسة طيف الامتصاص لثلاثة أنواع من أيونات المعادن بتراكيز مختلفة تجريبيا ونظريا. انموذج الفحص هو نموذج Gaius وذلك من أجل إيجاد أفضل منحنى مناسب والمعادلة التي تسيطر عليها مع هذا السلوك. والأيونات المعدنية الثلاثة هي (كلوريد النحاس $Cu\,Cl_3$، كلوريد الحديد Fe_2Cl_3، و كلوريد الكوبالت $Co\,Cl_3$) بتراكيز مختلفة هي (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3. اشتملت الدراسة الطيفية على طيف مرئي للأشعة فوق البنفسجية والفلورة لجميع تراكيز العينة المختلفة. تشير النتائج إلى العديد من القمم التي تظهر من طيف الامتصاص في التركيز العالي لجميع محاليل أيونات المعادن، كما استمرت قمم الامتصاص المتعددة حتى عند أدنى تركيز في محلول أيون الحديد. ويظهر طيف الفلورة اثارة كبيرة لقوة الاشعاع كانت ملحوظة لكل من Cu^{+2} و Co^{+2} و Fe^{+3}. من دراسة النمذجة، هنالك تقارب بين النتائج العملية والنظرية لطيف الفلورة لأيونات المعادن. علاوة على ذلك ، فإن التماثل والتقارب اللذين تم تعريفهما بـ (r^2) ، كان بمتوسط قيمة معدلها (0.995).

Introduction

Study the spectroscopy originally knows the interaction between radiations with the matter as a function of wavelength (λ). Traditionally spectroscopy referred to the use of visible light dispersed according to its wavelength [1]. On the other hand, spectroscopy represents a scientific measurement technique for the study of matter through its interaction with different components of the electromagnetic spectrum [2]. Metal ions are atom compounds that have an electric charge. Such atoms gladly miss one or more electrons to build positive ions called positive ions "cations". These ions are necessarily surrounded by delocalized electrons which are accountable for processes like electricity [3]. Metal ions are essential in biological processes such as photosynthesis process, and they can play a direct or indirect role in "biological processes", and helpful for clinical therapy processes, such as the use of "Lithium component" in the handling of bipolar disorder [4]. Also, follow up levels of metal ions in a variety of situations is necessary, like environmental following up and analysis of water, and in a wide variety of matrices, such as residue, soil, and water [5].

Metal ions prefer to connect with Oxygen centers, which are easily ready in numerous biological structures [6, 7]. Although positive ions "cations" of metal are important for several processes, the occurrence of the incorrect metal, or even the necessary metals in the erroneous concentration or position, can cause undesired consequences. They play a crucial part in determining the corroboration and stuffing of "nucleic acids" [8]. Binding of metal ions are interaction between proteins and metals, which can compose structural species. On the other hand, metal ions as Iron (Fe^{+3}), Cobalt (Co^{+2}), Chromium (Cr^{+3}) among others, are susceptive of confessing acceptor groups of electrons from the proteins that compose the complex structures [9, 10]. Furthermore, ionic liquids are amid the complexes that have been ahead of swelling acceptance. They are salts with a low melting point, commonly lower than room temperature [11]. An enormous number of different because of a large number of possible alterations of the positive ions, it can be produced ionic liquids. In addition to the nature of the ring and the difference of the side chain extension, play important roles in producing the ionic liquids [12, 13].

When classifying metals as important, copper can consider globally important metals. It is one of the most important metals used widely in several industrial types, military and microelectronic because of its typical electrical thermal conductivity, also it is good obtainability, affordability, and noble properties relatively [12, 14]. In recent years, it has been using nitrogen, oxygen, and sulfur to prohibit the oxidation from copper after many working cycles, these compounds are polar functional groups, and unify double bonds are usually utilized as restraint copper erosion during working [15-17]. Cobalt has been used since ancient times as a tool to give the color blue to ceramics and glass, also it is used as a base material in the manufacture of lithium batteries. It is also utilized radioactive signal and for the production of gamma rays with high energy [18, 19].

Many researchers investigated on activity and interaction of metal ions, some of them study the effect of metal ions on electrical properties [20]. Optical specifications and characteristics [21]. Another make improving the thermal properties of metals[22]. While some article shows the ability to use the metal as optical sensors [23]. Another's investigated the effect of metal ions on zeta potential [24] and the evolution of the structural and electrical properties of containing for the metal ion [25]. At the moment, some research dope the metal ions with some chemical compounds and study the influence on some physical properties [26, 27]. But most research absences a theoretical work that summarizes the behavior of the metal ions spectra to be a reference. That it can return to find out the behavior of metal ions in different cases.

In this paper, we study to examine the effect of concentration of three metal ions (Copper chloride, Iron chloride and Cobalt chloride) dissolved in ethanol. This effect was on absorption and fluorescence spectrum. Also give theoretical model for these effect, and find the best equation controls behavior of absorption and fluorescence spectrum for these metal ions with large range of concentration through limited conditions.

Experimental procedure

Copper chloride ($CuCl_3$) molecular weight (169.905 g/mol). Iron chloride (Fe_2Cl_3) molecular weight (218.049 g/mol). And Cobalt chloride ($CoCl_3$) molecular weight (165.29 g/mol) are dissolved in ethanol depending on their chemical formula by Eq. (1) [28]:

$$W = \frac{Mw * [M] * V}{1000} \quad (1)$$

where W is the weight of metal ion powder, V is the volume of ethanol, and Mw is the molecular concentration of the metal ion. The solution was diluted according to Eq. (2):

$$C_1V_1 = C_2V_2 \quad (2)$$

where V_1 and V_2 are the volumes of the liquids after and before dilution.
For all metal ions used in this work, the concentrations were (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

UV-Visible examination of samples is by "UV-Vis. spectrophotometer (Ultrospec. 4300 pro)". The fluorescence spectrum of samples is by fluorescence instrument "Jerelash grating 82-410, lmetff Gzemy- Tmer Spectumeter Spectogmph". The modeling part investigation is made by the Gaius model in 2D Table Curve "v5.01".

Results and discussion

1. Absorption spectrum

Fig.1 illustrated the absorption spectrum of Copper chloride with concentrations are (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3 respectively.

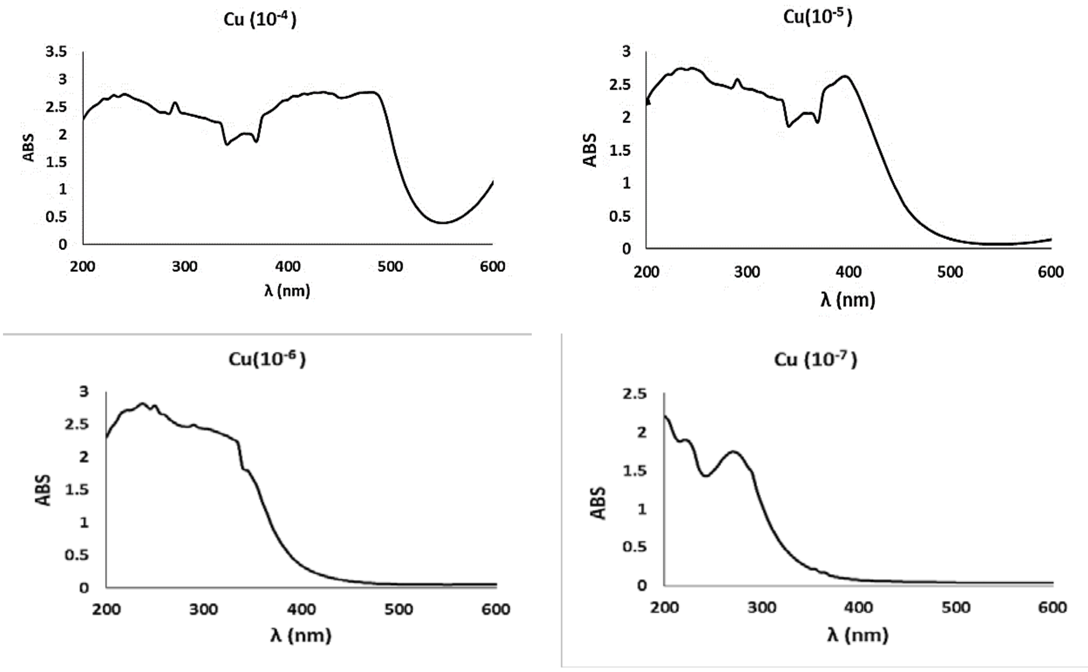

Fig.1: The absorption spectrum of Copper chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

Fig.2 illustrates the absorption spectrum of Iron chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3 respectively.

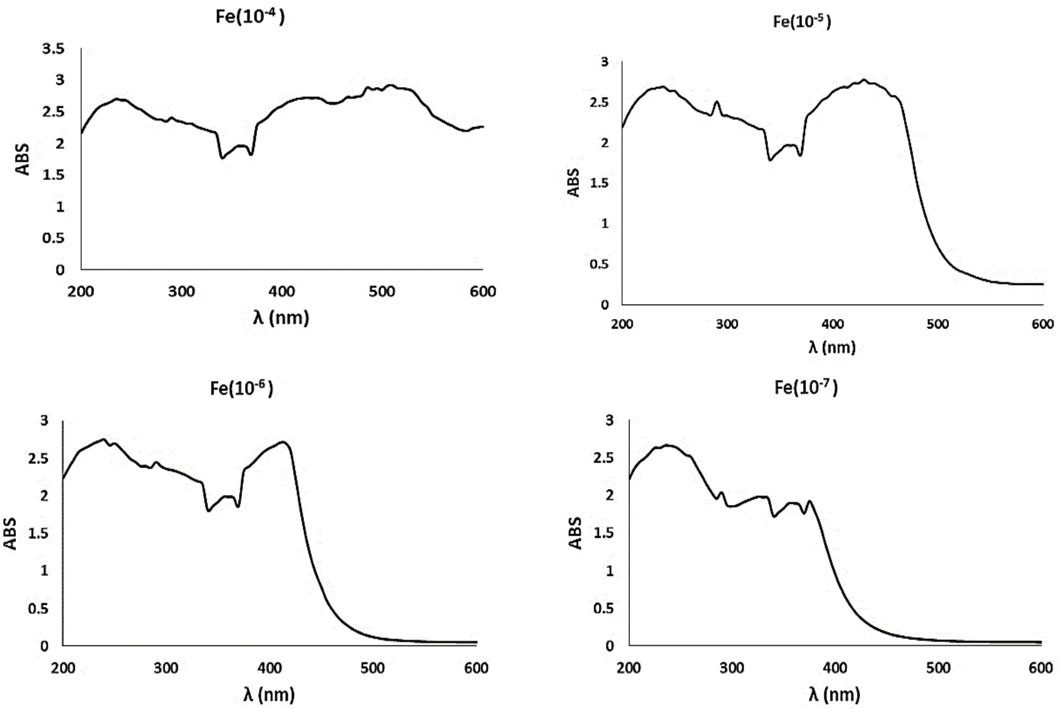

Fig.2: Absorption spectrum of iron chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

Fig.3 illustrates the absorption spectrum of Cobalt chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3 respectively.

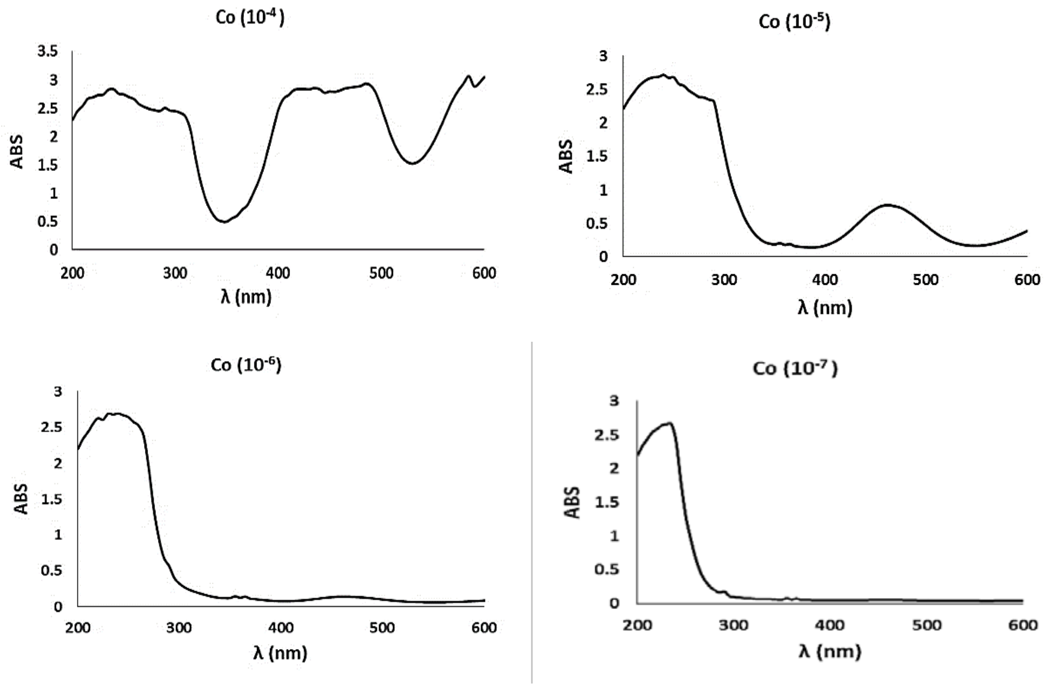

Fig.3: Absorption spectrum of Cobalt chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

Many peaks appear from the absorption spectrum of all metal ions solution, especially in high concentration (C). Since in high concentrations particle is in closet with another, leading to more trapped radiation (more light is blocked), "these are because the absorbance and concentration are directly proportional". If the original concentration is increasing, the absorbance increases, and if dilute the solution, the absorbance will decrease in direct proportion. In case of C=10^{-6} and 10^{-7} gm/m^3 highest absorption peak is one and clear in between 200-300 nm in Copper chloride, and at 250 nm in case of Cobalt chloride, while the multiple absorption peaks continued even at the lowest concentration used in the iron ion solution, this is because the oxidation of iron ion solution under UV radiation in the occurrence of iron chloride was experimental in the 1950s when it was postulated that the electron transmission started by radioactivity results in the generation of OH, responsible for the oxidation reactions [29, 30]. In these cases and for these reasons, it cannot study the absorption spectrum theoretically; the theoretical study was limited to the results of the fluorescence spectrum only.

2. Fluorescence spectrum

Fig.4 illustrated the fluorescence spectrum of Copper chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3 respectively.

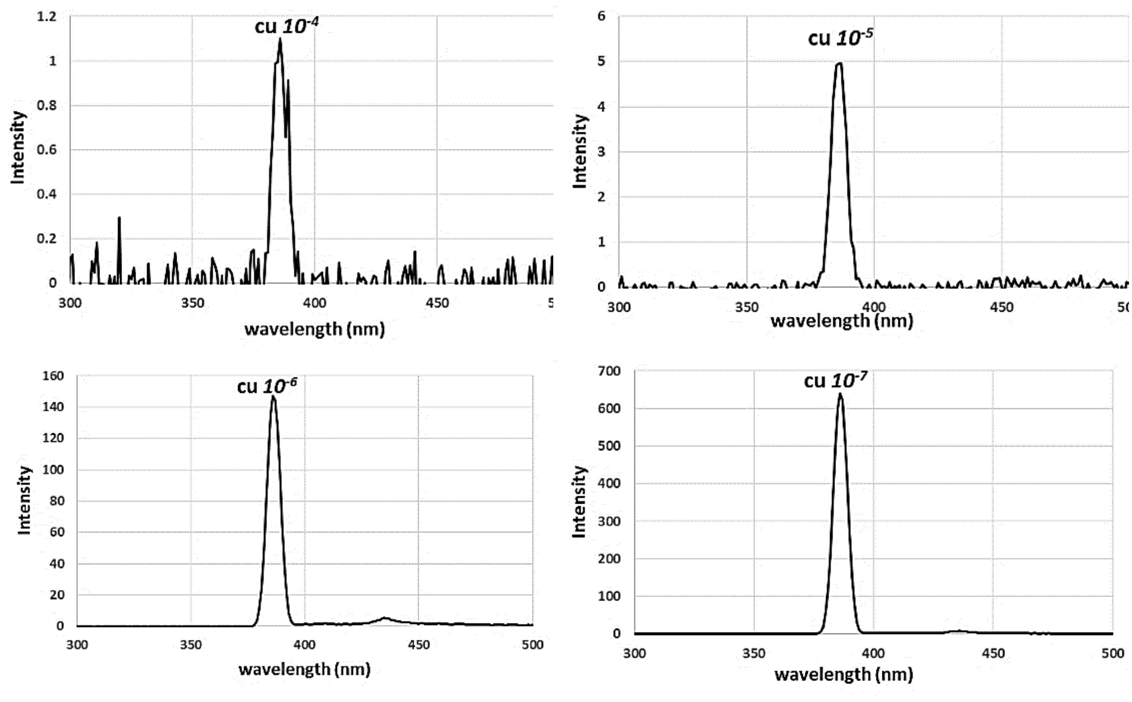

Fig.4: Fluorescence spectrum of Copper chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

Fig.5 illustrates the fluorescence spectrum of Iron chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3 respectively.

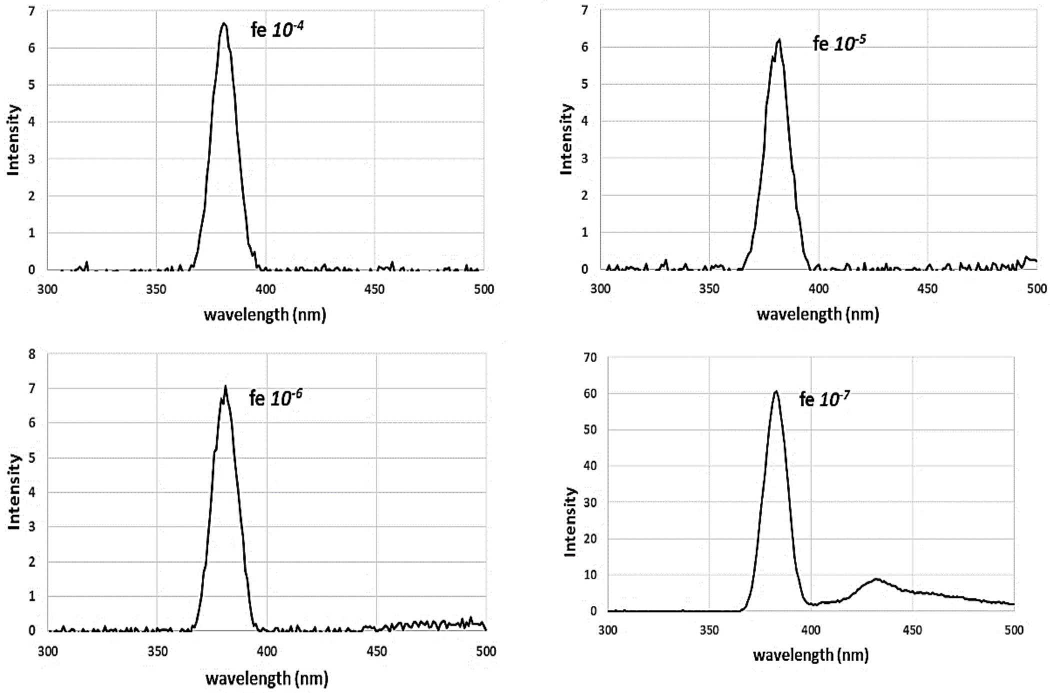

Fig.5: The fluorescence spectrum of Iron chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

Fig.6 illustrated the fluorescence spectrum of Cobalt chloride with concentrations are (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3 respectively.

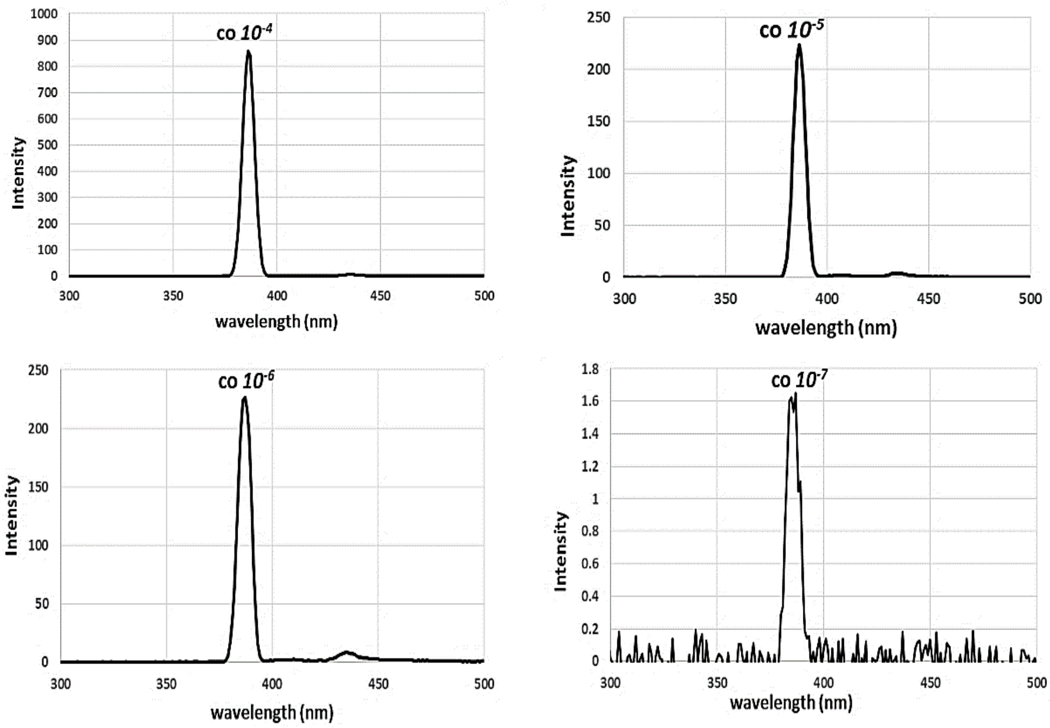

Fig.6: Fluorescence spectrum of Cobalt chloride with concentrations of (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

The fluorescence spectrum shows intensive stimulating of the radiation strength was perceived in the manifestation of Cu^{+2}, $Co^{+2,}$ and Fe^{+3}.

Because of the institution of a firmer "O-dansyl" electron donor instead of "HN-dansyl fluoro ionophores" which shifts coordination partialities for these transition metal ions. This results in strong complex formation with Cu^{+2}, Co^{+2} and Fe^{+3} [31]. In addition, these metal ions in nature are hard acids, compared to the other metal ions, in other hands, the positive metal ions are electron "pair acceptors", and can be considered as "Lewis acids". To duplicate, for example copper atoms themselves are not acidic or basic, but copper ions are acidic. So they will be attacked with oxygen to make strong compounds [32].

Modeling part

The theoretical investigation is made by the Gaius model in 2D table Curve "v5.01". This investigation was on the fluorescence spectrum only, because of the behavior of the absorption spectrum difficult and have several peaks. For all samples use the exponential function, since the using of it give the best approximation for sample's behavior, Figs.7-9 show the fitting curve of fluorescence spectrum for metal ions Cu^{+2}, Co^{+2} and Fe^{+3} respectively with different concentrations is (10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}) gm/m^3.

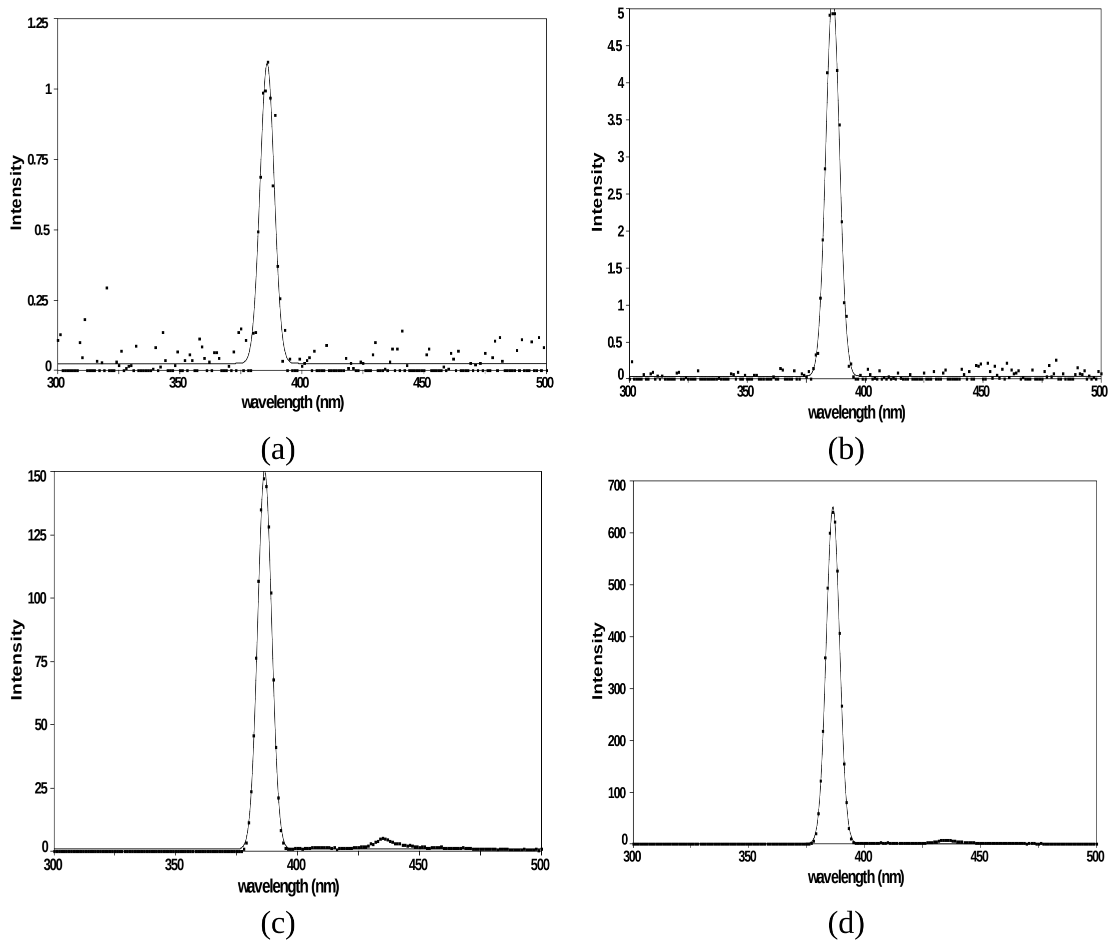

Fig.7: Fitting Curve of Copper chloride with concentrations of:
(a) 10^{-4}, (b)10^{-5}, (c)10^{-6}, (d)10^{-7} gm/m^3.

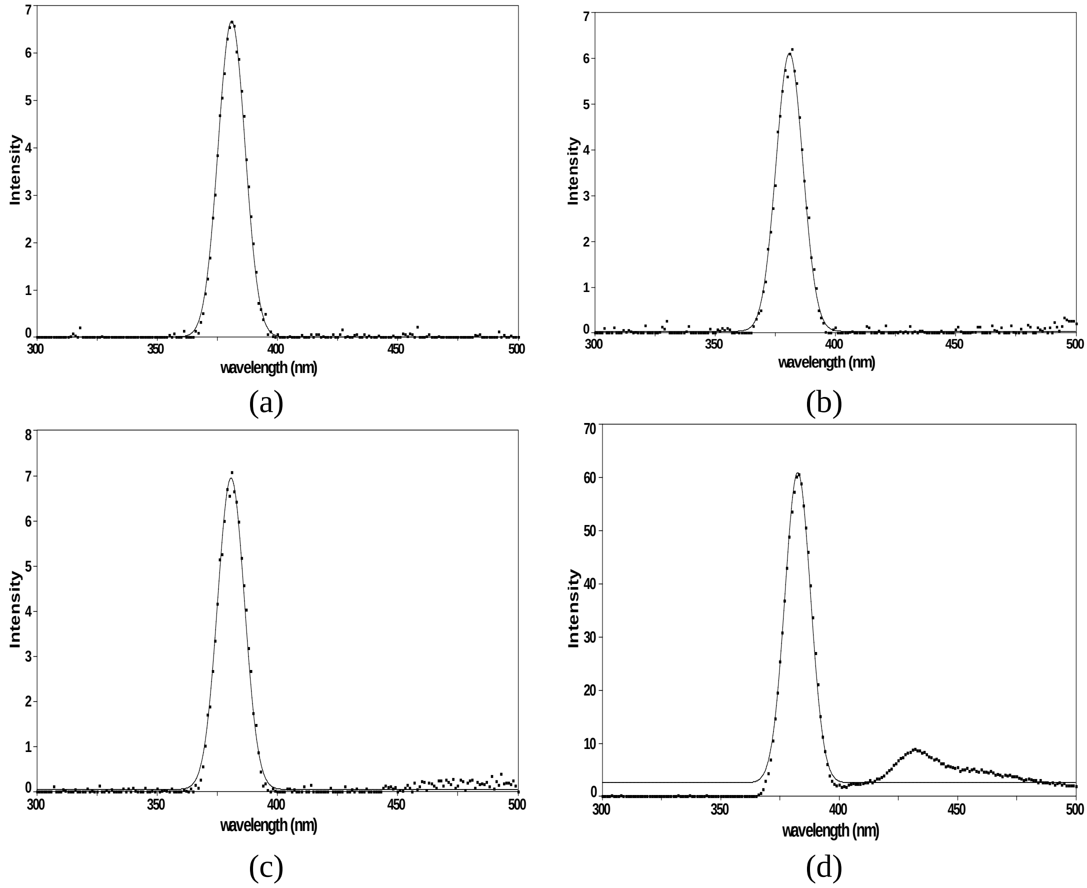

Fig.8: Fitting Curve of Iron chloride with concentrations of: (a)10^{-4}, (b)10^{-5}, (c)10^{-6}, (d)10^{-7} gm/m^{3}.

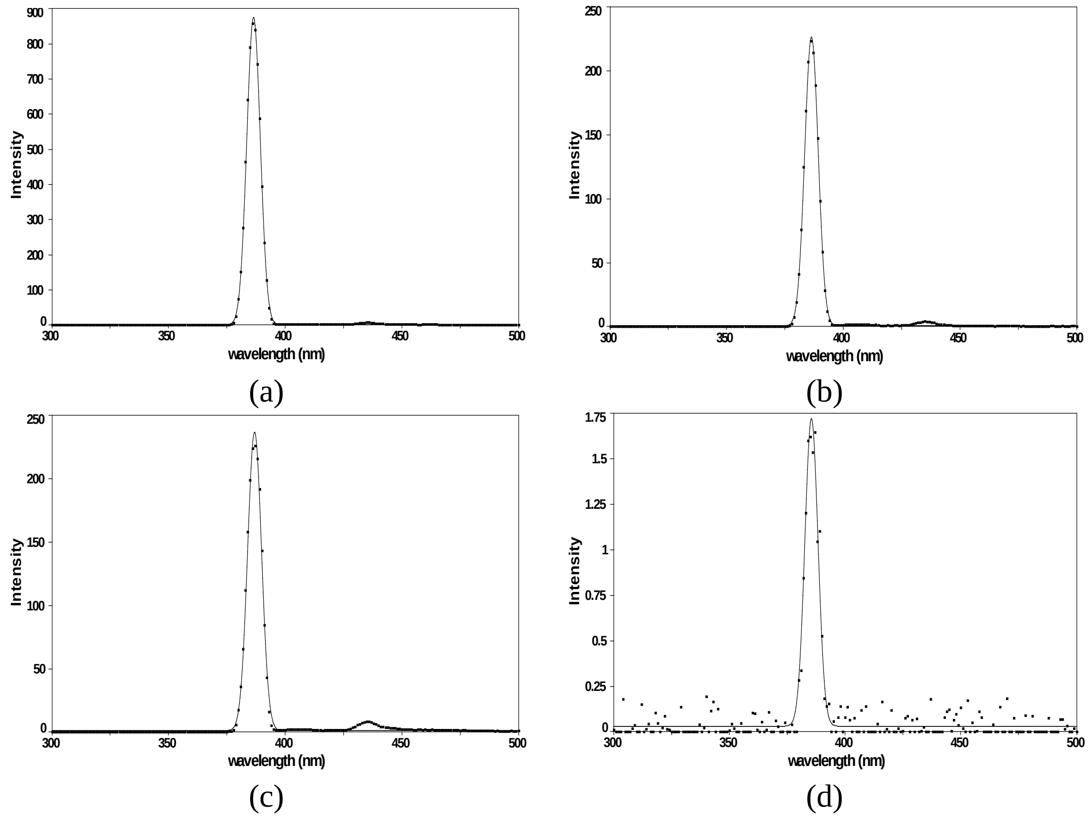

Fig.9: Fitting Curve of Cobalt chloride with concentrations of: (a)10^{-4}, (b)10^{-5}, (c)10^{-6}, (d)10^{-7} gm/m^{3}.

Figs.7-9 show there are converge between experimental and theoretical results of the fluorescence spectrum for metal ions. Furthermore, identity and convergence which defined as (r^2), are on average (0.995) as illustrated in Table 1.

Theoretical study enables us to refer to the function used (exponential function), and its application in a wide range of molar concentrations of metal ions that have been studied in this work, without resorting to preparation in practice again. So it can say there is the ability to use this fitting curve by the exponential function which following equation to give the best closer results between experimental and theoretical results fluorescence spectrum for metal ions.

$$y = a + b\exp(-0.5\left(\frac{x-c}{d}\right)^2) \qquad (3)$$

Table 1: Value of equation's coefficients and stander deviation error (StdErr) for Cu^{+2}, Co^{+2} and Fe^{+3} with different concentrations.

metal	concentrations	a	b	c	d	r^2	StdErr
Cu	10^{-4}	0.025	1.066	385.9	2.869	0.911	0.052
	10^{-5}	0.037	5.163	386.1	2.877	0.992	0.069
	10^{-6}	0.940	149.5	386.3	2.839	0.997	1.216
	10^{-7}	1.297	649.7	386.1	2.848	0.999	2.428
Fe	10^{-4}	0.010	6.666	381.0	5.586	0.998	0.062
	10^{-5}	0.039	6.072	381.0	5.564	0.995	0.088
	10^{-6}	0.058	6.891	380.8	5.562	0.994	0.112
	10^{-7}	2.586	58.37	382.6	5.408	0.960	2.492
Co	10^{-4}	1.205	874.4	386.3	2.884	0.999	3.233
	10^{-5}	0.634	226.1	386.2	2.877	0.998	1.134
	10^{-6}	1.289	235.8	386.7	2.970	0.995	2.595
	10^{-7}	0.031	1.690	385.5	2.826	0.951	0.059

Conclusions

Concentration is important rule in spectral properties of metal ions, this effect is apparent in the absorption spectrum particularly, until in low concentration this result attributed to the complex structure of them, and own many electrons in outer shell, as well as in high concentrations particle is in closet with another, leading to more trapped radiation means more light is blocked leading to several peaks in absorption spectrum, in the fluorescence spectrum at high concentration there are strong quenching of the radiation intensity were observed, because institution of a firmer "O dansyl" electron donor instead of "HN dansyl fluoro ionophores" which shifts coordination partialities for these transition metal ions.

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