

# Study of Thermodynamic Variables to Adsorption of Aldomete Drug (Methyldopa) from its Water Solution on the Nano Zinc Oxide Surface

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## ABSTRACT

The experiment was carried out to study the adsorption of aldomete on the surface of nano zinc oxide and its effectiveness in drug adsorption which causes poisoning in the case of doses exceeding the usual doses. UV spectroscopy technique was used to follow the concentration of the drug in the water solution after mixing it with 0.1 g of nano zinc oxide, and different solutions of the drug were used to obtain the adsorption isotherm and tested the applicability of the Langmuir and Freundlich equation for isotherm of the adsorption. The effect of temperature was investigated within the range (298 - 328) Kelvin and the best temperature was 298 Kelvin. The effect of time was also investigated within the range (30-180), and it was found that the largest amount of adsorption at time was 180 minutes. The adsorption was studied at pH = 1 and the thermodynamic functions ( $\Delta G$ ,  $\Delta H$ ,  $\Delta S$ ) were calculated, and the effect of ionic intensity on adsorption was studied by adding (0.1 M) of potassium chloride, it was found that the amount of adsorption of the drug on the surface of the nano zinc oxide increased with the presence of salt and showed the study of the ability of nano zinc oxide to adsorption the drug with highly efficiency.

**Keyword:** Aldomete drug, Nano zinc oxide, Adsorption, Thermodynamic.

## INTRODUCTION

The state of drug poisoning is produced when the drug is taken in a quantity above the dose or for long periods which sometimes leads to death<sup>1</sup>, and an effective way to treat cases of poisoning caused by excessive medication is the adsorption on the nano surfaces as a modern and effective means as these nanoparticles have distinct properties including high susceptibility to ion exchange<sup>2-5</sup> and high surface area which increase the pore size<sup>6,7</sup> which gives them the potential and high efficiency of adsorption of large molecules<sup>8,9</sup>, high absorption<sup>10</sup> and the lack of toxicity<sup>11</sup>, so we absorbed Aldomete drug on the surface of nano zinc oxide and It is a white powder to Insoluble in water<sup>12</sup>, It has a high stability in its physical and chemical properties<sup>13</sup>. So, it is used in many fields, including the ceramic industry<sup>14</sup>, pharmaceutical and cosmetic industries<sup>15</sup>, sensor industry<sup>16</sup>, electronics<sup>17</sup>, absorption of radiation and adsorption<sup>18</sup> and a catalyst as well as a non-toxic nature<sup>19</sup>. Aldomete drug is a scientific name is Methyldopa and it is one of the most common medications for lowering blood pressure, it is an antihypertensive medication and alpha-adrenergic receptor inhibitor, It is also an alpha-2-adrenergic receptor catalyst, and it works by stimulating the alpha receptors in the brain making it send nerve signals in the blood vessels which works to widen and relaxed it, leading to lower blood pressure, blood can flow easily through the body.

The chemical formula of the drug is (C<sub>10</sub>H<sub>13</sub>NO<sub>4</sub>), and its molecular weight (211.21g / mol). The structural formula as in figure (1), it is a crystalline powder of white to yellowish white or sometimes colorless crystals, it is odorless and tasteless, often dissolved in water<sup>20,21</sup>.

### Practical part

#### Devices used

The visible-UV spectrometer, type: Apple (PD-303 U.V.) Spectrophotometer Germany in Karbala University PH-Meter –WTW-720-ionlab Germany.

Thermostated Shaker Bath has a temperature controlled: Thermostated Shaker Bath, GFL (D-3006) Germany.

Centrifuge: Centrifuge, Megafuge 1.0, Herouse Sepatech, Germany.

Electric sensitive balance with four decimal places:

Electric Sensitive Balance, Sartorius medeian, Lab. BL 210 S, Germany.

### Materials used

Potassium chloride: KCl Fluka - Garantie, Switzeland

Hydrochloric acid HCl: BDH Chemical, ltd. poole, England

Aldomete drug: Iraq SDI

Nano zinc Oxides: Mknano, Mississauga, Canada.

### Work methods

Determination of the wavelength of the aldomete and calibration curve: To determine the maximum wavelength at which the highest absorption occurs. ( $\lambda_{max}$ ) The absorption spectrum of Aldomete was taken using the

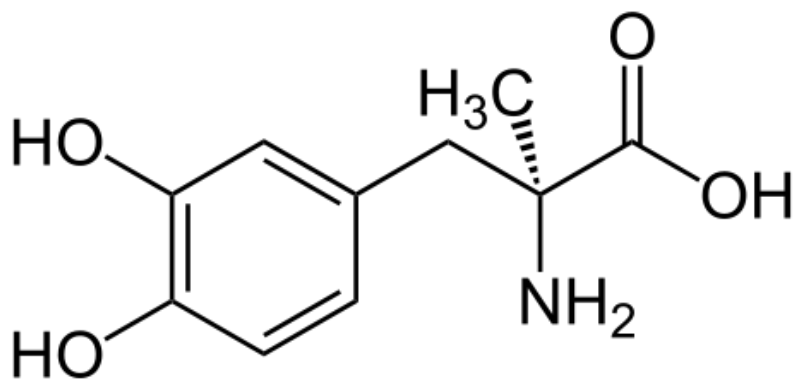
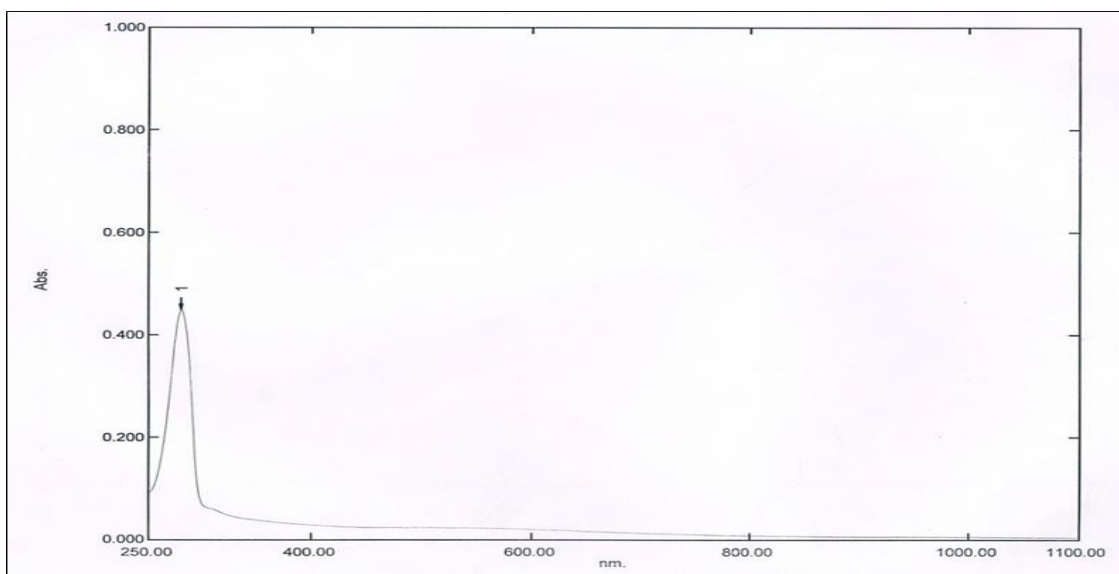
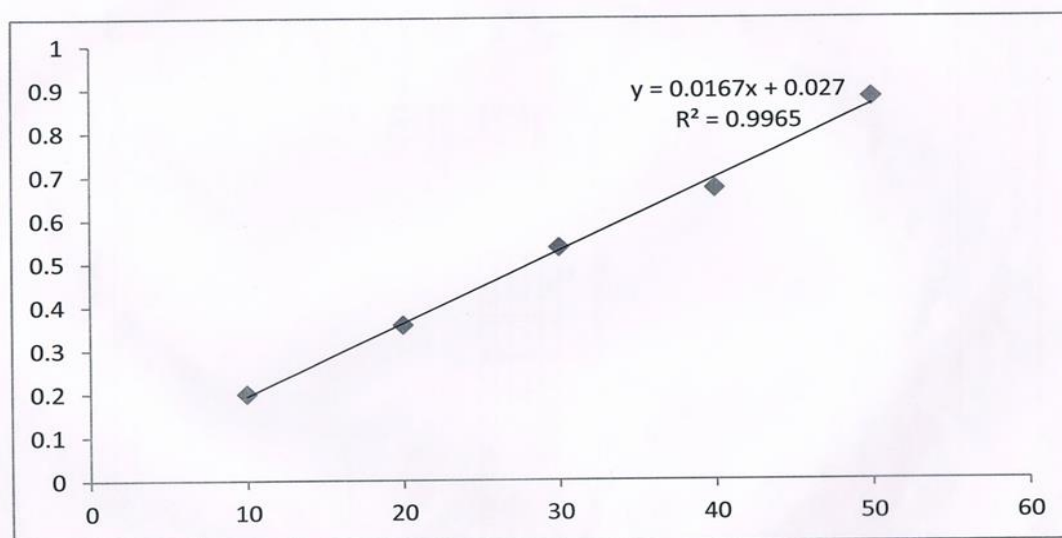


Figure 1: Structural formula of Aldomete drug.

Figure 2: UV spectrum of the Aldomete drug at  $\lambda_{\max}=280\text{nm}$ .Figure 3: Curved calibration of Aldomete solution at  $\lambda_{\max}=280\text{nm}$ .

UV-visible spectrometer within the range (250-1100) nm, and the maximum wavelength (280) nm as in Fig (2). The calibration curve, which represents the relationship between absorbance and concentration, was determined by

preparing five consecutive concentrations within the range of 10 - 50 ppm of the Aldomet solution used in the study. The absorbance of these concentrations was measured at the maximum wavelength ( $\lambda_{\max}$ ) Between

Table 1: shows log qe, log Ce values of aldomete drug on the surface of nano ZnO at pH = 1.

C <sub>0</sub> (mg/l)	Ce(mg/l)	Qe(mg/g)	Ce/ Qe	Log Ce	log Qe
10	6	1	9.33	0.845098	-0.12494
20	14	1.5	9.33	1.146128	0.176091
30	22	2	11	1.342423	0.30103
40	30	2.5	10.54	1.462398	0.439333
50	38	3	12.66	1.579784	0.477121

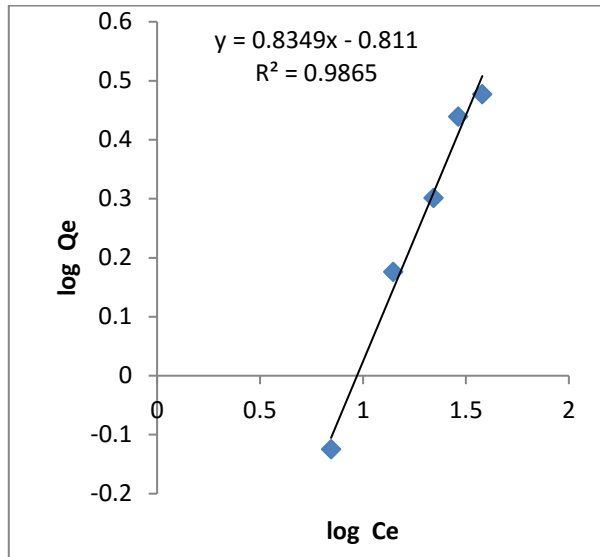


Figure 4: Freundlich straight to the adsorption of the drug on the surface of Aldomete on nano ZnO at temperature of 298 k and pH = 1

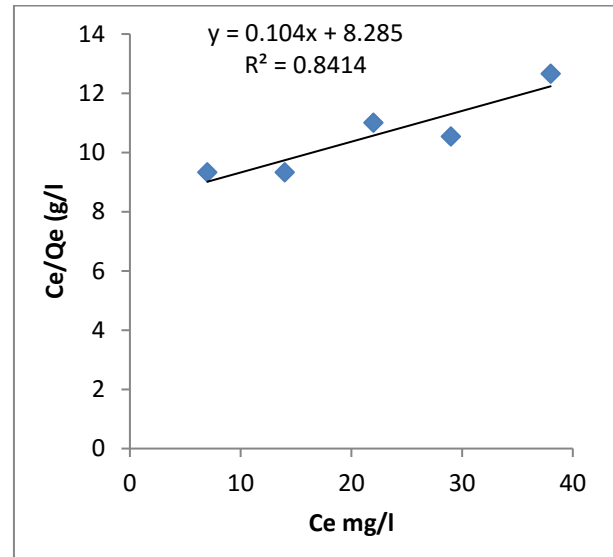


Figure 5: Langmuir straight to the adsorption of the drug on the surface of Aldomete on nano ZnO at temperature of 298 k and pH = 1

Table 2: shows the effect of temperature on adsorption of aldomete drug on the surface of nano ZnO in experimental range (298 -328) K.

C <sub>0</sub> (mg/l)	298 <sup>0</sup> K		308 <sup>0</sup> K		318 <sup>0</sup> k		328 <sup>0</sup> k	
	Ce (mg/l)	Qe (mg/g)	Ce (mg/l)	Qe (mg/g)	Ce (mg/l)	Qe (mg/g)	Ce (mg/l)	Qe (mg/g)
10	5.50	1.12	5.50	1.12	6.50	0.90	7.50	0.62
20	13.00	1.75	13.00	1.75	15.50	1.12	16.60	0.85
30	20.00	2.50	22.00	2.00	24.00	1.50	24.40	1.40
40	25.00	3.75	29.00	2.75	31.50	2.12	32.00	2.00
50	32.00	4.50	36.00	3.50	38.00	3.00	40.00	2.25

Table 3: Values of 1/ Tk and Log Xm for adsorption of Aldomete drug on the surface of nano ZnO in experimental range (298 - 328) K.

C <sup>o</sup>	Tk	1/Tk	Xm	Log Xm
25	298	0.003356	4.50	0.653
35	308	0.003247	3.50	0.544
45	318	0.003145	3.00	0.477
55	328	0.003048	2.25	0.352

absorption and concentration as shown in Figure (3).

*Determination of the equilibrium time*

To determine the equilibrium time between the solvent surface and the absorbent material, 0.1 g of nano oxide was put in contact with 25 mL of aldomete solution at a concentration of 10 bermalon at 303 kV and the absorbance was followed at different times

(30,60,90,120,150,180 minutes) And found that the equilibrium time of the drug 180 minutes.

*Adsorption isotherm*

The adsorption isotherms were determined by taking (0.1) g of nano zinc oxide surface in contact with 25 mL of the water solution of the drug for each concentration within the range (10-50 ppm) and then placed in a water bath

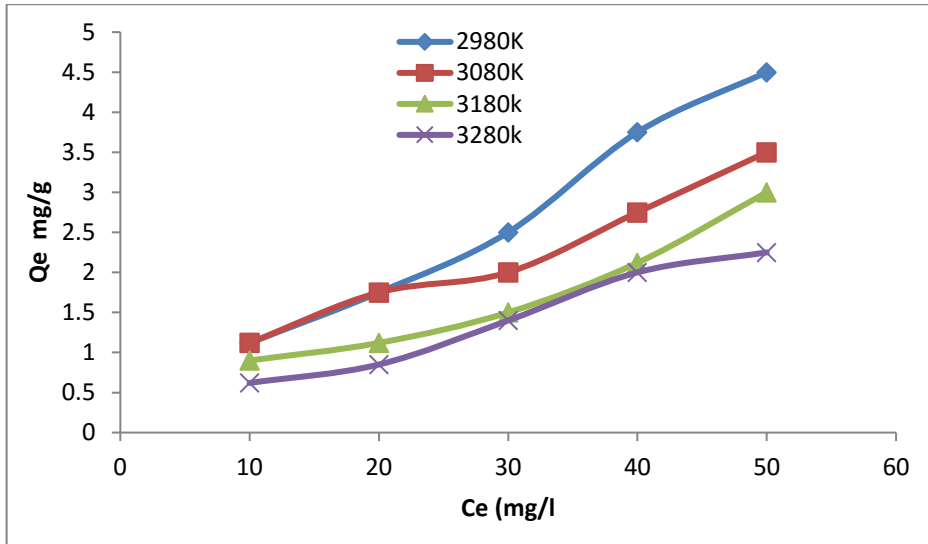


Figure 6: shows the effect of temperature on adsorption of aldomete drug on the surface of nano ZnO in experimental range (298 -328) K at PH=1.

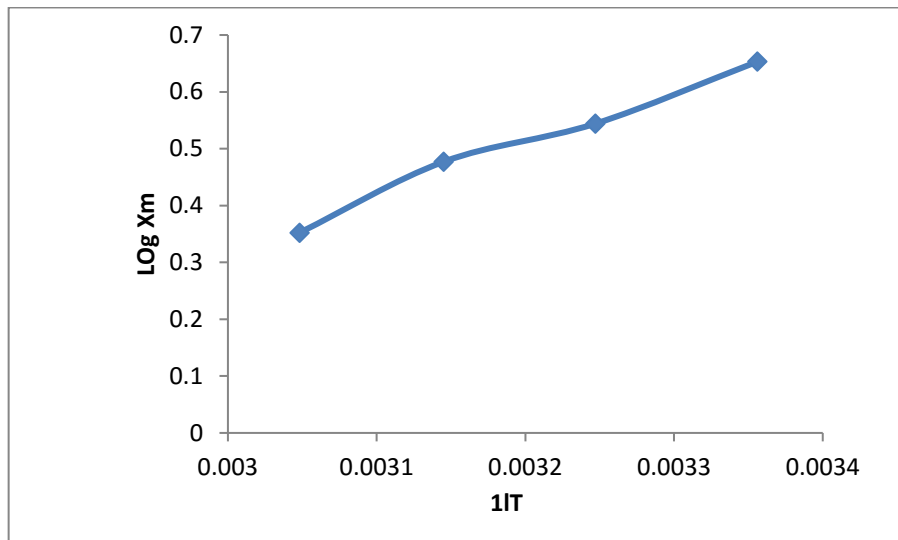


Figure 7: Log Xm vs. 1 / Tk of nano aldomete on ZnO surface

Table 5: Values of  $\Delta H$ ,  $\Delta G$  and  $\Delta S$  of aldomete on the surface of nano ZnO at a temperature of 298 K.

$\Delta H$ (KJ.mol <sup>-1</sup> )	$\Delta G$ (KJ.mol <sup>-1</sup> )	$\Delta S$ (J. mol <sup>-1</sup> )
-0.02	4.87	-3.72

with shaker and stabilized temperature at 298k. Upon reaching the pre-determined equilibrium time, The solution was then placed in the centrifuge at 3000 cycles per minute. The solutions were then filtered and measured using UV spectrometer. The quantity of the absorbent substance ( $Q_e$  / mg / g) was calculated according to the following relationship<sup>22</sup>.

$$Q_e = \frac{(c_0 - c_e) V_{sol}}{m}$$

Effect of temperature: For the purpose of studying the effect of temperature in adsorption isotherm study of drug adsorption isotherm in successive temperatures is (328,318,308,298) Kelvin.

Effect of ionic intensity

To study the effect of ionic intensity on adsorption, a concentration of potassium chloride (0.1M) was prepared and the isotherm adsorption study of the drug solution and compare them with the pharmaceutical solution that free of potassium chloride.

## RESULTS AND DISCUSSION

### Isotherms of the adsorption

A study of the adsorption of the aldomete drug from water solution on the surface of nano zinc oxide was conducted, and the corresponding absorbed quantity was calculated for each value of equilibrium concentrations at different concentrations and PH = 1, which represents the value of the optimal acid function of the stomach and a temperature of 298 K as adsorption of different forces on different parts of the surface. The adsorption capacity is also reduced by increasing the covered portion of the surface We observe that adsorption increases with increasing concentration of equilibrium<sup>23</sup> of the results

Table 6: Effect of time in aldomete drug adsorption on the surface of nano ZnO at 298 k.

Time (min)		30	60	90	120	150	180
50 ppm	Ce (mg/l)	38.80	38.00	30.50	28.80	27.60	25.30
	Qe (mg/g)	2.80	3.00	4.87	5.30	5.60	

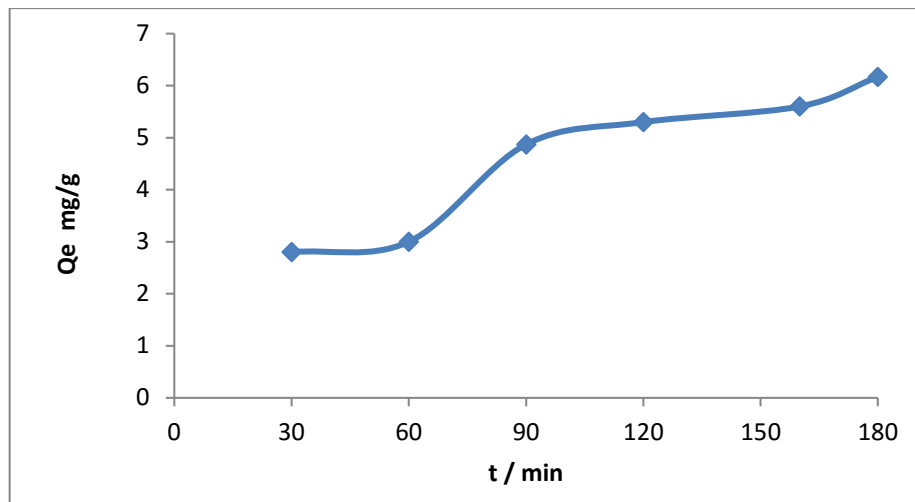


Figure 8: Effect of time in aldomete drug adsorption on the surface of nano ZnO at 298 k and at pH = 1 and contact time of 180 min.

Table 6: Effect of ionic intensity of aldomete drug adsorption on the surface of nano ZnO at 298 k and at pH = 1.

C <sub>0</sub> (mg/l)	With KCl (0.1M)		Without KCl	
	Ce (mg/l)	Qe (mg/g)	Ce (mg/l)	Qe (mg/g)
10	6	1	7	0.75
20	13	1.75	16	1
30	22	2	26	1
40	30	2.5	34	1.5
50	38	3	43	1.75

shown in Table (1) and Figure (4), it is observed that it follows the Freundlich equation to give it a linear image by drawing values (logQ<sub>e</sub>) against (logC<sub>e</sub>) and follow the Langmuir equation to give it a linear relationship when drawing (C<sub>e</sub> / Q<sub>e</sub>) against (C<sub>e</sub>) as in Figure (5).

*Effect of temperature*

A study of the effect of temperature in adsorption of aldomete drug on the surface of nano zinc oxide was conducted in the experimental thermal range (298-328) K. The results in Table (2) and Figure (6) indicate that the adsorption of the drug decreases by increasing the temperature and this applies with the thermodynamic properties<sup>24</sup>. The highest absorption was found at 298 K. And through the negative ΔH value, we find that the process is exothermic, this indicates that the process is only adsorption and it indicates that the adsorbed molecules that are diffused on the surface and are reduced the speed their diffusion, resulting in reduced interaction between the surface and the absorbed molecule.

As the temperature increases, the bonds will be separated<sup>25</sup>. HH is calculated from the log x<sub>m</sub> logarithm versus the inverted temperature of 1 / T as in Table 3 and Figure 7 according to the following equation<sup>26</sup>:

$$\text{Log } x_m = - \Delta H / (2.303 RT) + \text{conc} \dots\dots\dots (2)$$

A linear relationship was obtained as in Fig. (7). The value of ΔG was obtained from the following equation ΔG = -RT ln [ Q<sub>e</sub> / C<sub>e</sub> ] ..... (3)

The entropy values were obtained by the following equation:

$$\Delta G = \Delta H - T\Delta S \dots\dots\dots (4)$$

Table (4) shows the values of ΔH, ΔG and ΔS at different temperatures.

*Contact time*

The contact time has an effect on the adsorption of the dye on the surface of the nano zinc oxide to reach the contact state where placed (0.1) g of the surface in contact with 25 ml of dye at a concentration of 50 Ppm by taking ten flasks and placed these flasks in a water bath with a shaker and temperature stabilized at 298 K, and then the first flask was withdrawn after five minutes, and it was filtered and placed in a centrifuge and measured its absorbency, thus, for the rest of the flasks, work was done after every five minutes up to 180 minutes. It was noted that the time required for the equilibrium is (180) minutes to be (180) minutes, The mechanism of the reaction is explained by the migration and transfer of drug molecules from solution to surface. By the forces of distribution and dispersion until they reach equilibrium at the time mentioned<sup>27</sup> as in Table (6) and Figure (8).

*Effect of ionic intensity in adsorption*

*Effect of ionic intensity on the adsorption*

A study was conducted in the effect of ionic intensity in the adsorption on the surface of the nano magnesium oxide at 298 K for dye and pH = 1, Table (7) and Figure (9) show that the effect of adding KCl at a 0.1M concentration as a catalyst is that adsorption is more effective than if it is without salt. The adsorption of the

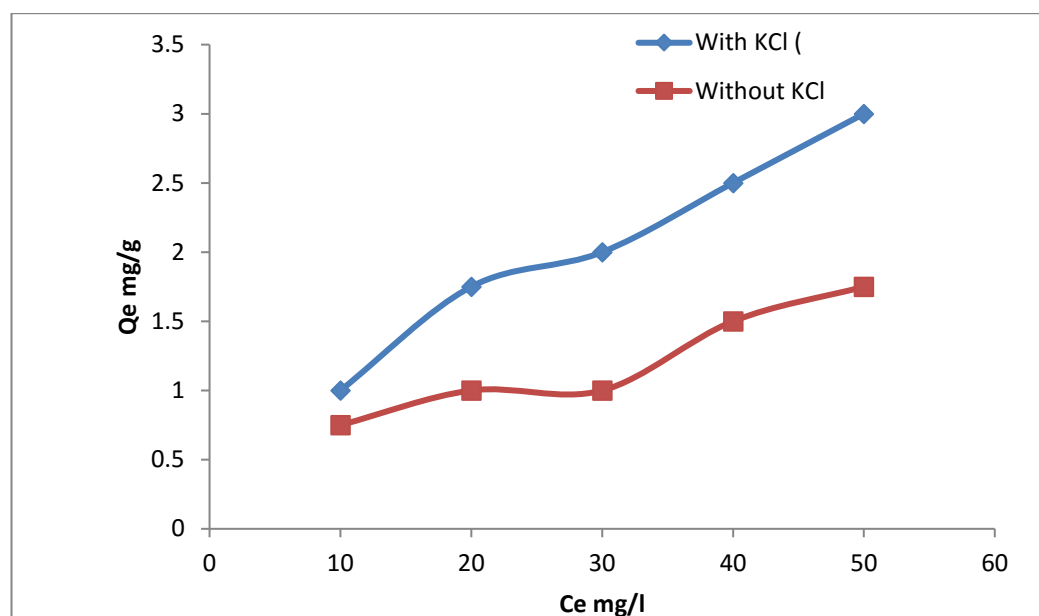


Figure 9: Effect of ionic intensity of aldomete drug adsorption on the surface of nano ZnO at 298 K and at pH = 1.

catalyst gives additional stability to the effective site versus the electrostatic interference<sup>28</sup>.

## CONCLUSIONS

Can benefit from the Nano zinc oxide to treat the poisoning of aldomete. It was found that the adsorption isotherm on the Nano zinc oxide followed Freundlich formula. The drug adsorption is exothermic and non-automatic. Adding salt increases the adsorption of the drug on the surface.

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