

Inhibitive effects of hydrochlorothiazide on the corrosion of aluminum 7075 in 0.1 M HCl and its adsorption characteristics

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Abstract

The corrosion inhibition effects and adsorption of 6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine -7-sulfo amide 1,1-dioxide [Hydrochlorothiazide (HYD) drug] on aluminum 7075 in 0.1 M HCl solution at 35 and 55 °C were investigated using weight loss measurements . It was found that the inhibition efficiency increased with the increase in HYD concentration .The temperature studies revealed an increase in the corrosion rate with an increase in temperature in the absence and the presence of the inhibitor .The thermodynamic parameters E_a , Q_{ads} and K_{ads} have been calculated . A mechanism of physical adsorption of HYD on the aluminum surface is proposed. The adsorption characteristics of inhibitor were approximated by Langmuir isotherm. The reactivity of the inhibitor was analyzed through quantum chemical calculations based on DFT methods at the B3YLP and 6-311++G (d ,p) basis set .

Key words: Aluminum, corrosion inhibitor, adsorption isotherm, Quantum chemical study.

1-Introduction

Al-Zn-Mg-Cu alloys have been widely applied to airplane structure due to their excellent mechanical properties, such as low density, higher elastic modulus and high ratio of strength to weight[1,2]. But they often suffered different type of corrosion such as intergranular corrosion , exfoliation corrosion and electrochemical corrosion , which can lower their strength, plasticity and fatigue properties, and decreases their service life [3, 4] .

An attempt to reduce electrochemical corrosion of aluminium , by isolate the metal from corrosion agents. This can be achieved by the use of corrosion inhibitors. Hydrochloric acid HCl solutions are used for pickling , chemical and electrochemical etching of Al⁽⁵⁾ and also used here as acid rain (pH 3.5 - 4.5) environment.

In recent years, owing to the growing interest and attention of the world towards environmental problems and towards the protection of environment and the hazardous effects of the use of chemicals on ecological balance , so the use of pharmacological substance -the major of it is natural products- as inhibitor for metals exposed to acid environment has continued to receive attention as replacement for synthesized organic inhibitor⁽⁶⁻⁸⁾.

It has been shown that the inhibitory action of the drugs used as inhibitors act through a process of surface adsorption, so the efficiency of an inhibitor depends not only on the characteristics of the environment in which it acts, the nature of the metal surface and electrochemical potential at the interface, but also on the structure of the inhibitor itself, which includes the number of adsorption active centers in the molecule, their charge density, the molecular size, the mode of adsorption, the formation of metallic complexes and the projected area of the inhibitor on the metal surface^(9,10).

The Hydrochlorothiazide (HYD) which is the object of the present investigation is non-toxic, cheap and environmental friendly diuretic drug. It contain reactive centers like N ,S ,O atoms which containing lone pairs , Cl and aromatic rings with delocalize electron systems which can aid their adsorption onto metal surfaces. Furthermore, they have high molecular weights and are likely to effectively cover more surface area (due to the adsorption) of the metal thus preventing corrosion from taking place. Thus, the present study was undertaking the corrosion inhibitive abilities of Hydrochlorothiazide Fig.[1] on aluminium alloy 7075 in hydrochloric acid solution using weight loss method at 35 and 55°C. Quantum chemical

calculations were further employed to explain the efficiencies of the compound as corrosion

inhibitors.

2. Experimental

The experiments were performed with aluminum 7075 sheets (which are used in aircraft industry)

having the chemical composition shown in table (1).

Table(1): Chemical composition in weight percent of Aluminium alloy 7075.

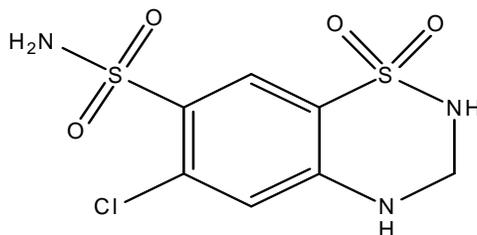
Metals	wt%
Cu	1.196
Mg	1.608
Mn	0.0430
Si	0.0975
Zn	5.308
Fe	0.135
Cr	0.1845
Ni	0.0069
Cd	0.002
Al	Bal.

Each sheet was 0.2 cm in thickness and was mechanically press-cut into coupons of dimension 2cm X 1cm . These coupons were used with further polishing. They were ,however, degreased in absolute ethanol, dried in acetone, and stored in moisture-free desiccators prior to use ⁽¹¹⁾.

All reagents used were BDH and Fluka analytical grade. They were used as sourced without further purification. An aqueous solution of 0.1 M HCl was used as a blank solution. Hydrochlorothiazide (HYD) , was purified using the procedures described in the literature^(12,13), which were added to the acid in concentrations ranging from 2×10^{-4} – 1×10^{-3} M. Experiments were conducted in the test solutions for 24 h progressively for 168 h (7 days) at 35 and 55 °C .

In each experiment, the cleaned aluminium coupon was weighed and suspended with the aid of glass rod and hook in a beaker containing 100 ml of 0.1 HCl. The coupon was then taken out of the test solution, washed in 70% nitric acid for 2 minutes to

remove the corrosion products using bristle brush, rinsed with distilled water, dried and reweighed. The weight loss was taken as the difference between the weight at a given time and the initial weight of the test coupon determined using Sartorius 120 digital balance with sensitivity of ± 0.1 mg. The tests were performed in duplicate to guarantee the reliability of the results and the mean value of the weight loss is reported. Weight loss allowed the calculation of the mean corrosion rate in miles per year (mpy). Complete geometry optimization of the HYD is performed using DFT (density function theory) with the Beck's three parameter exchange function along with the Lee-Yang-Parr non-local correlation functional (B3YLP)⁽¹⁴⁾ with 6-311++G(d ,p) basis set implemented in Gaussian 03 fully version program ⁽¹⁵⁾. This approach was shown to yield favorable geometries for a wide variety of system .This basis set gives good geometry optimization.



6-Chloro-3,4-dihydro-2h-1,2,4-benzo thiadiazine-7-sulfo amide 1,1-dioxid

Fig. [1]: The chemical structure of Hydrochlorothiazide (HYD).

3. Results and discussion

3.1 Inhibition efficiency

Weight loss of aluminium alloy 7075 were determined after 168 h (7days) of immersion in 0.1M HCl in the absence and the presence of various concentrations of Hydrochlorothiazide (Hyd) at 35 and 55 °C respectively.

The corrosion rate (CR)in (mpy) unite , was calculated from the following equation⁽¹⁶⁾:

$$CR = C \times \frac{m_1 - m_2}{area \times t} \times K \quad \dots\dots(1)$$

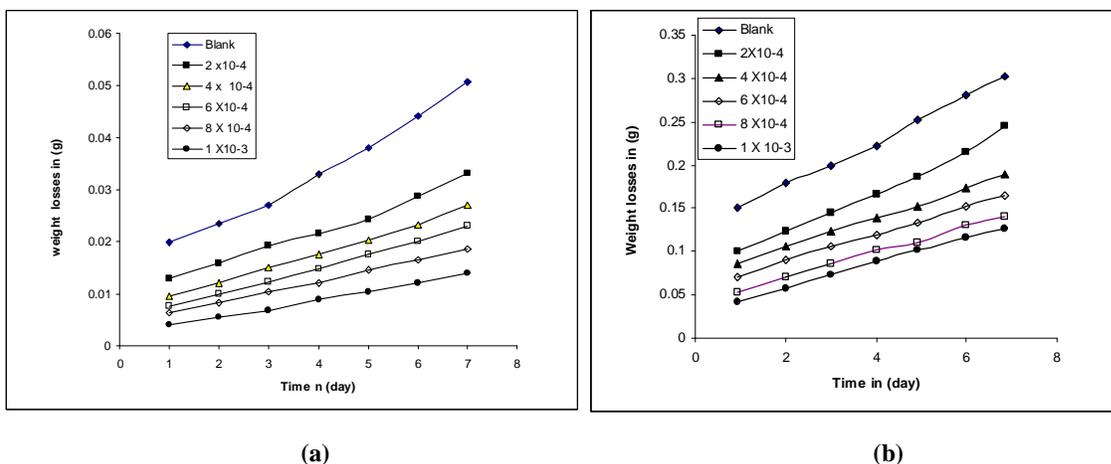
where m_1 and m_2 are the mass of the aluminum 7075 coupon before and after immersion in (mg)respectively , C is constant equal to (437), the area of the alloy coupon in (cm^2), t is the corrosion time in (hours) and K is a density factor which equal to 2.81 for aluminum 7075. The calculated corrosion rate (CR) in equation (1) is an average corrosion rate as no localized corrosion takes place

.The percentage inhibition efficiency (%IE) was calculated by using corrosion rates with the following equation⁽¹⁷⁾:

$$\% IE = [CR_0 - CR] / CR_0 \times 100 \quad \dots (2)$$

where CR_0 and CR are the corrosion rates of the aluminum 7075 coupon in 0.1 M HCl in the absence and the presence of (HYD) respectively.

Fig.[2a] shows a representative plot of weight loss against time (days) for aluminum 7075 in 0.1 M HCl in the absence and the presence of different concentrations of HYD at 35°C. Similar plots were obtained for 55 °C Fig.[2 b]. The figures clearly shows a reduction in weight loss of the metal coupons in the presence of the inhibitor compared to the blank.



Figure[2]: Plots of weight loss against immersion time for HYD at (a) 35°C and (b) 55°C.

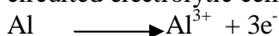
Table (2) shows the calculated values of corrosion rates obtained using equ. (1) as well as inhibition efficiency values evaluated using the expression given in equ. (2). It is clearly seen from the table that the corrosion rates were reduced in the presence of HYD compared to the absence for aluminum 7075 corrosion in 0.1 M HCl. Also the corrosion rates were observed to increase with the increase the temperature both in the absence and

the presence of inhibitors. Corrosion rates values are also seen to decrease with increase in concentration of inhibitor. This actually shows that the addition of HYD to the acid solution retards the corrosion rate of aluminum 7075 and that the extent of retardation is concentration dependent. Similar observations have been documented by several authors[18, 19].

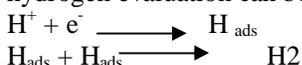
Table (2): Corrosion parameter for Al-alloy7075 in 0.1 M HCl in the absence and the presence of different concentrations of Hydrochlorothiazide (HYD) at different temperature

Inhibitor	System/concentration	Corrosion rate (mpy)		(% IE)	
		35°C	55°C	35°C	55°C
Hyd	Blank	71.123	424.493		
	2 x 10 ⁻⁴	46.666	344.37	34.386	18.87
	4 x 10 ⁻⁴	38.092	281.025	46.442	33.761
	6 x 10 ⁻⁴	32.329	231.925	54.545	45.3578
	8 x 10 ⁻⁴	26.143	196.785	63.325	53.642
	1 x 10 ⁻³	19.678	177.106	72.332	58.278

According to the electrochemical theory of corrosion, the anodic dissolution of Al in acidic solutions correspond to equation below in the short-circuited electrolytic cells .



While the reaction to the cathodes which lead to hydrogen evaluation can be represented as ;



Inhibition efficiency as given in Table (2) is found to increase with the increase in HYD concentration which indicates that more HYD components are adsorbed on the aluminum 7075 surface at higher concentration, leading to greater surface coverage, but IE% values decreased with the increase in temperature . Similar to the observations had been obtained in the previous work [20]. Inhibition efficiency increases with inhibitor concentration to reach 72.332 % for HYD at 1 x 10⁻³ M.

3.2 Adsorption isotherm

Since the corrosion inhibition process is based on the adsorption of the inhibitor on the metal surface, It is essential to know the mode of adsorption and the adsorption isotherm that fits the experimental results.

The most frequently used adsorption isotherms are Langmuir, Temkin and Frumkin with the general formula

$$f(\theta, X) \exp(-2a\theta) = KC \dots\dots\dots(3)$$

Plots of the obtained data for each isotherm showed that the of the investigated compound agreed with the Langmuir isotherm Fig.[3]that is given by [23]:

The inhibition efficiency observed for HYD may be explained by the presence of three nitrogen atoms with lone pair of electrons, which serve as adsorption centers for their interaction with the metal surface. On the other hand, four oxygen groups and phenyl group ,Also the presence of halogens such as (Cl)have been known to deactivate benzene rings [21].

The decrease in inhibition efficiency with an increased in the temperature as observed in present study (Table 2) for HYD suggested the physisorption mechanism that usually attributed to electrostatic interaction between charged molecules and the charged metal. This observation has been explained to be due to the reduction in stability of adsorbed film at higher temperatures.As temperature increases, Gibbs free energy and enthalpy rises to a high value, so that some of the chemical bonds joining the molecules onto the metallic surface are impaired and film stability reduced [22].

$$\frac{C}{\theta} = \frac{1}{K_{\text{ads}}} + C \dots\dots\dots(4)$$

where K_{ads} is the adsorption equilibrium constant, C is the concentration of inhibitors and θ is the coverage degree.

To calculate the surface coverage; θ, it was assumed that the inhibitor efficiency is mainly due to the blocking effect of the adsorbed species and hence

$$\theta = \frac{\%IE}{100} \dots\dots\dots(5)$$

The gravimetric results were used to calculate the adsorption isotherm parameters; because it can be assumed that adsorption equilibrium is established within 24 h.

The value of K_{ads} is related to the standard free energy of the adsorption, ΔG°_{ads} , by the following equation [24]

$$K_{ads} = \frac{1}{55.5} \exp\left(\frac{\Delta G^{\circ}_{ads}}{RT}\right) \dots\dots\dots(6)$$

where R is the gas constant and T is the absolute temperature. The value of 55.5 is the molar concentration of water in solution expressed in mol¹.

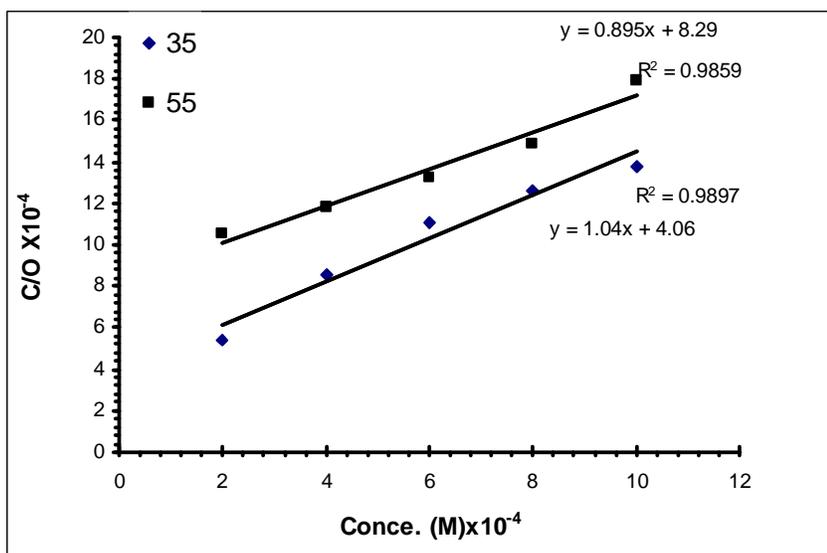


Figure [3]: Langmuir adsorption for HYD at 35 and 55°C.

The values of adsorption constant, slope, and linear correlation coefficient (R^2) can be obtained from the regressions between C/θ and C , and the results are listed in Table (3). The results showed linear correlation coefficients and the slopes are more than one at 35°C. So, it could be concluded that HYD unit occupies more than one adsorption site on the aluminium surface isotherm, and confirms that the adsorption of HYD in 0.1 M HCl follows the Langmuir adsorption isotherm. The thermodynamic parameters for adsorption process obtained from Langmuir adsorption isotherms for the studied inhibitor are given in Table (3) The negative values of ΔG°_{ads} reveal the spontaneity of

adsorption process and they are characteristic of strong interaction and stability of the adsorbed layer with the aluminum surface.

Generally, the ΔG°_{ads} values of -20 kJ mol^{-1} or less negative are associated with an electrostatic interaction between charged molecules and charged metal surface, physisorption; those of -40 kJ mol^{-1} or more negative involve charge sharing or transfer from the inhibitor molecules to the metal surface to form a coordinate covalent bond, chemisorptions [25]. The calculated ΔG°_{ads} value, being less than -40 kJ mol^{-1} indicates physical adsorption.

Table (3): Calculated thermodynamic parameter for HYD from Langmuir adsorption isotherm

Inhibitor	Temperature(°C)	K(M ⁻¹)	ΔG° (KJ/mol)	Slop	R ²
Hyd	35	2500	-32.288	1.075	0.9859
	55	1190	-28.419	0.8	0.9897

Also from Table (3) , it could be found that the equilibrium constant of the adsorption process (K_{ads}) decreased with increasing temperature. It is well -known that K_{ads} designates the adsorption power of inhibitor onto the aluminium surface. Clearly, HYD gave high values of K_{ads} at lower

temperatures, indicating strong adsorption on the aluminium surface. Thus, the inhibition efficiency decreased with the increase in temperature as a result of the desorption HYD from the aluminium surface.

3.3 Effect of temperature on the inhibition characteristics of HYD

To assess the effect of temperature on corrosion and corrosion inhibition processes, gravimetric experiments were performed at 35 and 55°C. The apparent activation energies (E_a) for the corrosion process in the absence and the presence of the inhibitors were evaluated from a modified form of the Arrhenius equation:

$$\log \frac{\rho_2}{\rho_1} = \frac{E_a}{2.303R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \dots\dots\dots(7)$$

where ρ_1 and ρ_2 .are the corrosion rates at temperature T_1 and T_2 respectively, and R the molar

gas constant. An estimate of heat of adsorption Q_{ads} was obtained from the trend of surface coverage at different temperature as follows [26]:

$$Q_{ads} = 2.303R \left[\log \left(\frac{\theta_2}{1-\theta_2} \right) - \left(\frac{\theta_1}{1-\theta_1} \right) \right] \left(\frac{T_1 \times T_2}{T_2 - T_1} \right) \dots (8)$$

Where θ_1 and θ_2 are the degrees of surface coverage at temperatures T_1 and T_2 , The calculated values for both parameters are given in Table(4).

Table (4): The values of activation energy (E_a)and heat of adsorption (Q_{ads}) for 7075 alloy dissolution in 0.1 HCl in the HYD at 35 and 55°C

System/concentration	E_a (kJmol ⁻¹)	Q_a (kJmol ⁻¹)
Hydrochlorothiazoid(HYE)		
Blank	7.502	
2 x10 ⁻⁴	8.393	-32.777
4 x10 ⁻⁴	8.392	-12.224
6 x10 ⁻⁴	8.275	-15.174
8 x10 ⁻⁴	8.477	-16.635
10 x10 ⁻⁴	9.227	-26.403

The higher value of E_a in the presence of HYD compared to that in the absence and the decrease of their %IE with temperature increase can be interpreted as an indication of physical adsorption.

The negative Q_{ads} values obtained for HYD indicate that the degree of surface coverage decreased with theirise in temperature, supporting the earlier proposed physisorption mechanism .

3.4 Mechanism of corrosion inhibition

The adsorption of HYD onto the aluminium surface is found to be majorly physical in nature. Physical adsorption can occur by electrostatic attraction between charges or dipoles of the adsorbed species and the electric charge on the metal surface which can be expressed by the value of pH_{zch} , which is defined as the pH at a point of

zero charge, which is equal to 9.1 for aluminium [27] so aluminium surface is positively charged at pH 1, which is the pH value of 0.1M HCl solutions that were used in this investigation. Thus the addition of HYD molecular , can also be present as protonated species in an acid solution So, it can be

concluded that HYD can be adsorbed onto aluminium surface in two different ways:

(i) The protonated inhibitors electrostatically adsorb onto the anion covered aluminium surface, through their protonated form .

3.5 Quantum chemical studies

Through these calculations an attempt has been made to correlate corrosion inhibition efficiency (dependent variable) and the set of some independent variables like frontier molecular orbitals (HOMO) highest occupied molecular orbital which is used to predict the adsorption center of the molecules, lowest unoccupied molecular orbital (LUMO) ,number of overall electrons ,dipole moment etc[28]. . The geometry was optimized

(ii) The inhibitors compete with acid anions for sites at the water covered surface and adsorbed by donating electrons to the aluminium.

using DFT method at the level of B3LYP and 6-311++G(d,p) basis set.

Geometric and electronic structure of the HYD was calculated by the optimization of their bond lengths, bond angles table (5) and dihedral angles. The optimized molecular structures with minimum energies obtained from the calculations are shown in Fig.[4] .

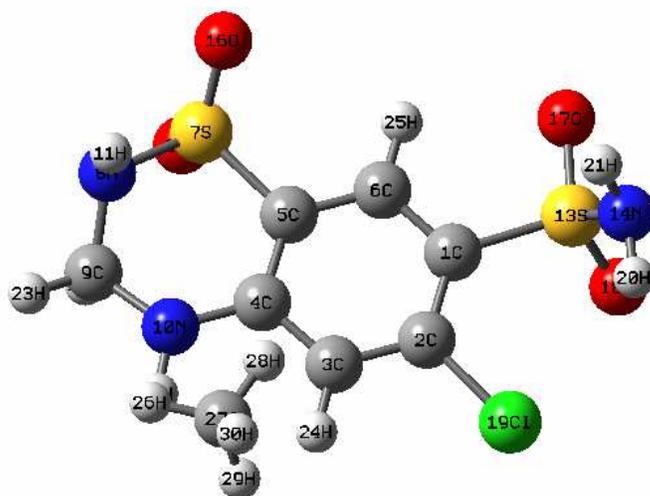


Figure [4]: The optimized molecular structure of HYD.

Table (5): Selected structural parameters (bond lengths and bond angles) of HYD molecules

Atoms	Bond distance (Å)	Atoms	Bond distance (Å)	Atoms	Bond angles (°)
C1-S13	1.813	S7-O15	1.455	C2-C1-S13	124.5
C2-C119	1.752	S-O16	1.454	C6-C1-S13	117.2
C3-C4	1.408	N8-C9	1.453	C1-S13-S14	107.8
C4-C5	1.413	C9-N10	1.464	C3-C4-N10	120.0
C4-N10	1.375	S13-N14	1.671	C5-C4-N10	122.6
C5-S7	1.795	S13-O17	1.456	C4-C5-S7	120.0
N8-S7	1.695	S3-O18	1.453	C4-N10-C9	122.0

It is shown from the geometrical structure parameter of HYD Table(5) that the C5–S7 bond has the longer bond length, 1.795 Å compared with the C4-N10 bond length 1.375 Å which indicate the strain found in the HYD molecules. Also the dihedral angle between the atoms N8S7C5C4 and C9N8S7C5 equal to 20.118 and -49.841 respectively which leads to non planer HYD molecules so the surface coverage cannot be as uniform as is observed for planner molecules. The highest bond order of S-O shown in Table (4)

indicates a double bond character of this type of bonds.

The calculated Mulliken charge table(6) shows that the N,O and some C atoms has a negative charge, where the C9 atom has high electron density(-0.494) and S atoms have an electron deficient,. This means that the N8,N10,N14 , and all the oxygen and the carbon which has negative charge could be considered as an active adsorption center towards the metal surface.

Table (6) : The Mulliken charges (Q_M) atoms

Atoms	Mulliken charges
C1	-1.325
C2	0.496
C3	-0.624
C4	-0.137
C5	-0.202
C6	-0.113
S7	0.747
N8	-0.289
C9	-0.494
N10	-0.121
S13	0.257
N14	-0.372
O15	-0.138
O16	-0.126
O17	-0.151
O18	-0.05
C19	0.492

E_{HOMO} is a quantum chemical descriptor which is often associated with the electron donating ability of the molecule. High value of E_{HOMO} likely indicates a tendency of the molecule to donate electrons to appropriate acceptor molecule of low empty molecular orbital energy. Therefore, E_{LUMO} indicates the ability of the molecule to accept electrons. So, the lower the value of E_{LUMO} , the more probable the molecule accepts electrons [29]. The binding ability of the inhibitor to the metal surface increases with the increase in the HOMO and the decrease in the LUMO energy values.

The calculated quantum chemical parameters show that the inhibitor has the HOMO and the LUMO orbital energies at -7.114 and -2.055 eV ,

respectively. Accordingly, HYD has the highest separation energy, ΔE , 5.059 eV which means the highest reactivity of the inhibitor towards the metal surface and hence the good inhibition efficiency. Also, the calculations show that it has the highest dipole moment, 10.523 D, which increases the adsorption on the metal surface.

Molecular orbital calculations are performed to calculate the molecular orbital coefficients of the HOMO and the LUMO levels for the investigated HYD inhibitor to explain the mechanism of adsorptions on the metal surface. The HOMO electronic density distribution for the HYD is plotted in Fig. [5]

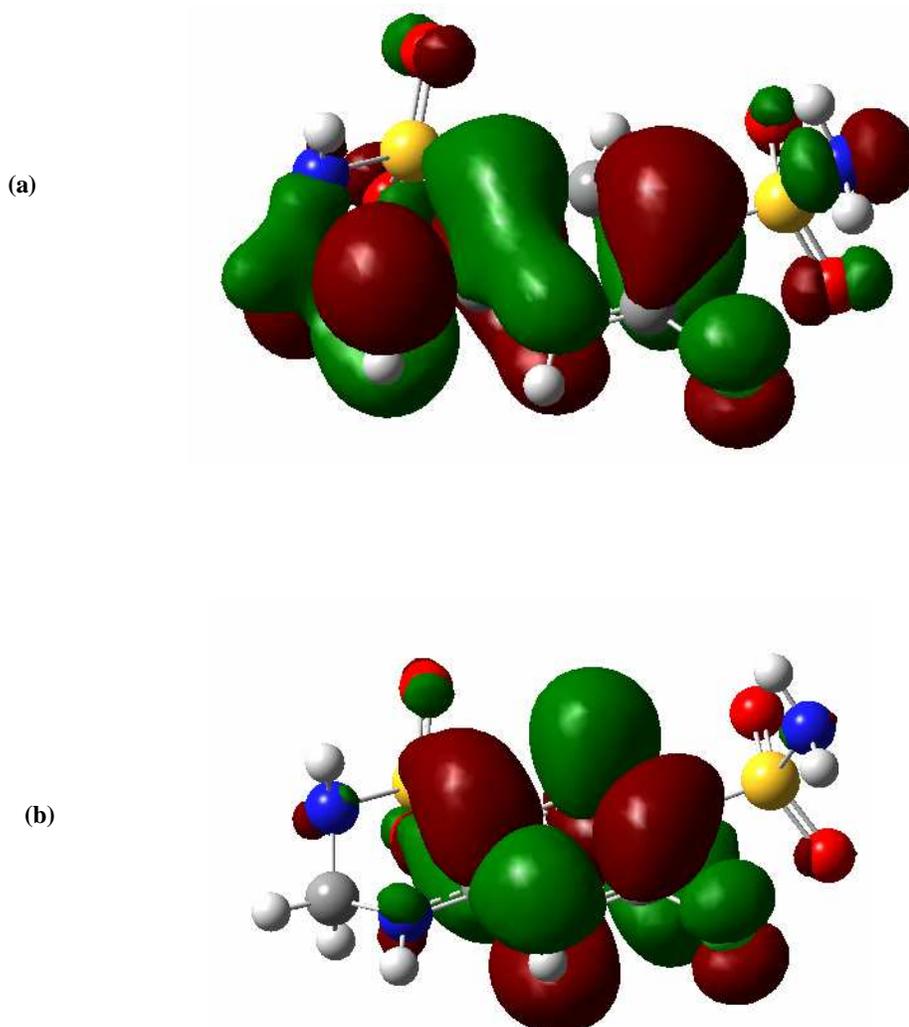


Figure [5] : The three dimensions picture of (a) Highest Occupied Molecular orbital (HOMO) ,(b) The Lowest Unoccupied Molecular Orbital (LUMO) of the inhibitors

It is shown from the calculations that the highest coefficient in the HOMO level can be represented as localization of charge density on the nitrogen atoms, oxygen atoms and delocalization of the charge on the other moieties. Accordingly, the adsorption on the metal surface can occur through the lone pair of electrons of the nitrogen, the lone pair of electrons of the oxygen atom, and the π charge of the other moieties which increase the adsorption centers of HYD and increase its inhibition efficiency.

In the case of the LUMO level with complete π^* character, the charge is mostly localized on the phenyl group which facilitates the back donation from the metal surface to the anti-bonding character of the inhibitor. This indicates that the inhibitor binds strongly with the metal surface and accordingly increases its inhibition efficiency. Meanwhile, the adsorption of HYD on the metal surface could be explained as electron donation from the inhibitor molecule to the metal surface and back donation from the d-orbital of the metal surface to π -anti-bonding counterpart of the inhibitor.

References

- 1- G. S. Chen, M. Gao, R.P. Wei; *Corrosion*, 52, 8, (1996).
- 2- Y. L. Cheng, Z. Zhang, F. H. Cao, J. F. Li, J. Q. Zhang, J. M. Wang and C. N. Cao ; *Mate. and Corr.* , 54, 601–608 (2003)
- 3- Christian Vargel "*Corrosion of Aluminum*" , Elsevier (2004).
- 4- F. M. Khoshnaw and R. H. Gardi ; *Mate. and Corr.* , 58, No. 5,(2007).
- 5- M. Abdallah ; *Corr. Sci.*, 50,1981-1996,(2004).
- 6- M.S.Morad ; *Corr. Sci.*, 46,436-448,(2008).
- 7- N. O. Eddy, S. A. Odoemelam and P. Ekwumemgbo; *Scientific Research and Essay* , Vol. 4 (1), 033-038, (2009).
- 8- Sudhish K.Sukla and M. A. Quraishi; *Corr. Sci.* , 51,1007-1011 , (2009).
- 9- M .M .El-Naggar ; *Corr. Sci.*, 49,2226-2236 , (2007).
- 10-I.B.Obot, N.O .Obi-Egbedt and S.A.Umoren ; *Int. J. Electrochem. Sci.* , 4 , 863-877,(2009).
- 11- A.O.James, N.C.Oforka ,O.K.Abiola and B.Ita ; *Ecl.Quim* , 32 , 3 , 31-38,(2007).
- 12- AdilA.Al-Fregi and Haider A.Abood; *J. Basrah. Research Science*,3,31-41,(2004).
- 13- Haider A.Abood ; *Basrah J of Sci. C*, 24 ,1,48-67,(2006).
- 14- A.D..Becke; *J. chem. Phys.* ,96,9489,(1992).
- 15- M.J. Frisch, et al. ; **Gaussian 03, Revision C.02**, Gaussian, Inc.,
- 16- R.Babolan"*Corrosion tests and standard Application and Interpretation* " ASTM manule series :MNL20 2nd Edition
- 17- O.Krim,M.Bouachrin,B.Hammouti , A.Elidrissi and M.Hamdi; *Prot. Electrochmi. Acta*;26,283-289(2008).
- 18- T.Jain,R.Chowdhary and S.P.Mathur ; *Mate. and Corr.* ,57,5,(2006).
- 19- A.Fouda,A.A,AL-Sarawy,F.Ahmed and H.M.El-Abbasy; *Corr. Sci.*,51,485-492,(2009).
- 20- N. O. Eddy, S. A. Odoemelam and A. J. Mbaba ; *African Journal of Pure and Applied Chemistry*, 2 ,12,, 132-138 ,(2008).
- 21- P.Mthews;"*Advanced Chemistry*" Cambridge University Press , Great Britain ,(1996).
- 22-S.A.Umoran,I.B.Obot,N.O.Obi-Egbedi; *Mater. Sci.* ,44,1,27,(2009).
- 23-A.P.Samide and I.Bibicu ; *Surf. Interface Anal.* , 40 , 944-952 , (2008).
- 24-M.Behpour,S.M.Ghoreishi,N.Soltani and M.S.Niasari; *Corr. Sci.* , 51,1073-1082,(2009).
- 25-N.O.Eddy and S.A.Odoemelam; *Adv. in Nat. App. Sci.* ; 2,3,225-231,(2008).
- 26-P.M.Natisan , E.Mccaferty and G.K.Hubber ; *J. Electrochem.Soc.*, 133 10, (1986) .
- 27- K.Bahrara ,H.Kim and G.Singh; *Corr. Sci.* ,50,2747-2757,(2008).
- 28- G.Gece ; *Corr. Sci.* , 50,2981-2991,(2008).
- 29- H. Wang, X. Wang, H. Wang, L. Wang, A. Liu; *J. Mol. Model.* 13, 147, (2007).

تأثير تثبيط التآكل وخصائص الامتزاز للهيدروكلوروثاياوزويد على سبيكة الألمنيوم 7075 في 0.1 مولاري من حامض الهيدروكلويك

الخلاصة :

درس في هذا البحث تأثير تثبيط التآكل و الامتزاز لعقار هايدروكلوروثاياوزويد أو 6-كلورو -3,4-داي هايدرو 2H - 1, 2, 4- بنزو ثايا دايزين - 7 سلفونومايد 1،1 - داي وكسيد ،على سبيكة الألمنيوم 7075 في وسط من حامض الهيدروكلوريك 0.1 مولاري و عند درجتى 35 و 55 مئوية باستخدام طريقة فقدان الوزن .وقد تبين ان كفاءة التثبيط تزداد بزيادة تركيز هايدروكلوروثاياوزويد ،كما ان دراسة تغير درجة الحرارة تؤدي إلى زيادة معدل التآكل في حالة وجود و غياب المثبط مع انخفاض كفاءة التثبيط عند زيادة درجة الحرارة. كما حسبت أيضا العوامل الترموديناميكية لعملية الامتزاز مثل طاقة التنشيط و ثابت التوازن و انتالبي الامتزاز . أثبتت الدراسة ان المثبط يمتز على سطح المعدن بميكانيكية فيزيائية . تخضع لمعادلة Longmuir isotherm . كما استخدمت طريقة DFT /B3YLP من الميكانيك الكمي وبواسطة 6-311++G(d,p) basis set لغرض تفسير فعالية المثبط.

