

The study of the inhibitory properties of Omeprazole on the corrosion of Aluminum 6063 in alkaline media

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Abstract

The influence of (6-Methoxy-2-(4-methoxy-3,5-dimethyl-pyridin-2-yl-methanesulfinyl) or Omeprazole(OME) on the corrosion of aluminum 6063 in 2M NaOH solution has been studied using hydrogen evolution (gasometry) measurement at 30 and 55 °C temperature. The results suggest that OME acts as a good inhibitor and the inhibition efficiency increases with increasing the concentration of OME. The %I decrease with increase in temperature from 30 to 55°C in the absence and the presence of inhibitor and halides. The adsorption of inhibitor followed Temkin adsorption isotherm and the value of ΔG_{ads} , E_a , and Q_{ads} values suggests that it is physical adsorption. The synergism parameters (S_I) obtained were found to be greater than unity between I^- , Br^- , Cl^- ions and OME, which indicates that the enhanced inhibition efficiency caused by the addition of halides is only due to synergism. Some quantum chemical parameters and the Mulliken charge densities for OME were calculated by the semi-empirical AM1 method to provide further insight into the mechanism of inhibition of the corrosion process.

Key words: Aluminum; Corrosion inhibition; Adsorption isotherm; acid; Synergism; Halide ions, quantum chemical studies , Austin Model (AM1) .

Introduction

Aluminum depends on the presence of natural surface oxide film for its high corrosion resistance in several media, but alkaline solutions are known to render the oxide film non-protective; because OH^- ion dissolves the protective oxide and the

aluminum surface establishes a very negative potential (Olusegun et al., 2008 ; Zhanget al.,2009 ; Rosliza et al., 2010). Aluminum–alkaline solution systems are often utilized in the development of metal/air batteries in which the aluminum is used as the anode.

(Pyun et al., 2000). Another common example of aluminum–alkaline solution systems can be found in nuclear water reactors during a loss of coolant accident (LOCA). The chemical environment generated by the injection of coolant into the emergency-core-cooling-system has a pH around 10 (Klasky et al., 2005).

Several workers (Frenier et al., 1993 ; Philip et al.,2008; Abdel-Gaber et al.,2008) have employed organic and inorganic compounds as corrosion inhibitors to control this oxide film dissolution and thereby reducing the rate of metal loss in alkaline solutions. Inorganic compounds such as chromate ,dichromate ,nitrate are widely used as corrosion inhibitors in several media and for different metals and alloys(Fontana ,1986). On the other hand ,the biotoxicity of these product ,especially chromate ,is well documented (Vargel ,2004)as well as their non-environmental –friendly characteristics (Vargel ,2004), which limit their application.

Attention has been focused on the corrosion inhibiting properties of drugs (Shukla et al., 2010 ; El-shafei et al.,2004 ; Shukla et al.,2009;Shukla et al.,2010) because of its advantages over the use of some organic inhibitors , due to their eco-environmental nature , and the structure contains one or more polar function(with N,O and S atoms),in addition to heterocyclic group and π - electrons . The inhibition action of this

organic –drug - compounds is usually attributed to interaction with metallic surfaces by adsorption . The polar function is frequently regarded as the reaction center for the adsorption process establishment (Lowmunkhong et al.,2010).

This paper reports the effect of anti-inflammatory drug[6-Methoxy-2-(4-methoxy - 3 ,5-dimethyl-pyridin-2-ylmethanesulfinyl)-1H-benzoimidazole] or Omeprazole(OME)on the corrosion of aluminum 6063 in 2M NaOH using the hydrogen evolution technique at 30 and 55°C . The effect of different halides (KCl, KBr, and KI) on the efficiency of the OME is also being investigated to determine synergism , and theoretical calculation to the structure of drug using semi-empirical methods at AM1 levels were also studied.

Experimental details

Aluminium sheets of the type AA 6063(which are used in an electrical connections between towers and also due to its availability) having the chemical composition given in Table (1) were used in this study. Each sheet was 0.14 cm in thickness was mechanically press-cut into coupons of dimension 5 cm x 4 cm. These coupons were used as cut without further polishing. They were however degreased in absolute ethanol, dried in acetone, and stored in moisture-free desiccators prior to use (Ashassi et al.,2006)

Table (1): Composition in (wt%) of aluminum 6063

Wt%									
Si	Fe	Cu	Mn	Mg	Zn	Ti	Cr	Ni	Al
0.4830	0.1799	0.0008	0.0083	0.4051	0.0165	0.0145	0.004	0.0047	98.83

Omeprazole (OME) (6-Methoxy-2-(4-methoxy-3,5-dimethyl-pyridin-2-yl-methanesulfinyl)-1H-benzimidazole) was purchased from medicine shop as a trade name Omprazol-20 capsules, and used with further purification (Moffat et al., 1986; Marshall, 1988; Commission, 2006). Figure (1) shows the molecular structure of Omeprazole.

All reagents used were BDH analytical grade. They were used as sourced without further purification. An aqueous solution of 2 M NaOH was used as a blank solution. OME was added to the base in concentrations ranging 200 ppm to 600 ppm. The halide salts, potassium iodide, potassium bromide and potassium chloride was used in the concentration 0.05M for the synergistic studies.

The apparatus and procedure for hydrogen evolution method, 100 ml of the corrodent (2M NaOH) was introduced into the reaction vessel and Al 6063 coupons placed in it, and the reaction vessel was quickly close to prevent any escape of gas. The volume of hydrogen gas evolved was monitored as a function of time by measurement of the depression (in ml) in the

color water level. The same experiment was repeated in the presence of inhibitor (OME), halides and OME-halides mixtures. Results recorded are average values of three separate determinations.

The quantum chemical calculations were performed with gaussian03 program, semi-empirical method were using at the AM1 levels (Frishet al., 2004). The following quantum chemical indices were considered: the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}), $\Delta E = E_{LUMO} - E_{HOMO}$, dipole moment (μ), and Mulliken charges of OME. It is obvious that one OME molecule contains two nitrogen molecules with lone pairs of electrons that can serve as adsorption centres, and a lot of p electrons exist in this molecule making it suitable for this study (Figure(1)).

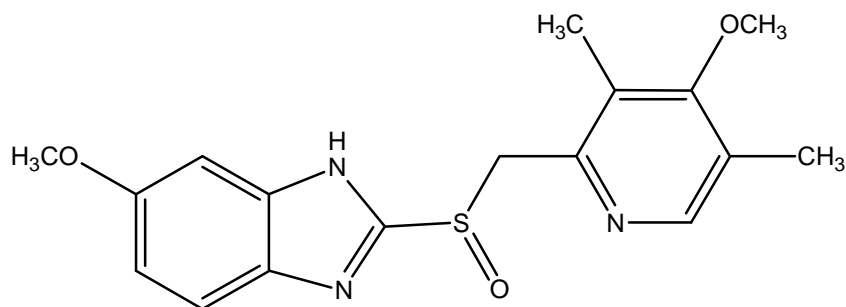
Results and discussion

a) Hydrogen evolution and corrosion rates

The relative rapidity and effectiveness of hydrogen evolution (gasometric) technique, as well as its suitability for monitoring in situ, any perturbation by an inhibitor with respect to gas evolution in metal/corrodent systems

have been established by earlier reports (Onuchukwu,1988 ; Oguzie,2007). Several authors have reported on comparable agreement between gasometric technique and other techniques of corrosion monitoring.

These include polarization measurement (Eltra ,2001), weight loss Mercier et al.,2009), and thermometric technique (Olusegun et al., 2009).

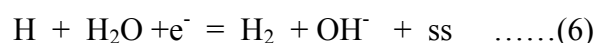
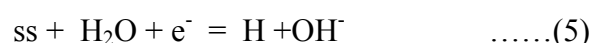
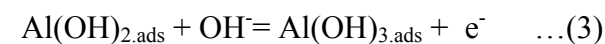
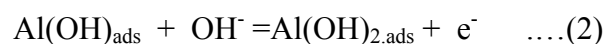


6-Methoxy-2-(4-methoxy-3,5-dimethyl-pyridin-2-yl-methanesulfinyl)-1H-benzimidazole

Figure(1): The structure of the inhibitor used in this study.

The corrosion process of Al in alkaline solution could be explained on the basis that the surface of Al is covered by passive film. When immersed in alkaline solutions, the outer surface of the film will dissolve, on the other hand, Al atoms in substrate will diffuse toward surface, or oxygen toward substrate, and combine to form passive film (Loreenzet al., 1981). In some areas, the passive film is not very dense due to structural defects and is relatively more soluble where its dissolution is faster than its formation. In these areas, dissolution of Al atoms and gradual removal of these atoms through the formation of hydroxide with increased coordination number from 1 to 3 to form independent molecular species of $\text{Al}(\text{OH})_3$ (see Eqs. (1)–(3)) takes place. $\text{Al}(\text{OH})_3$ species react in a pure chemical manner to form a soluble

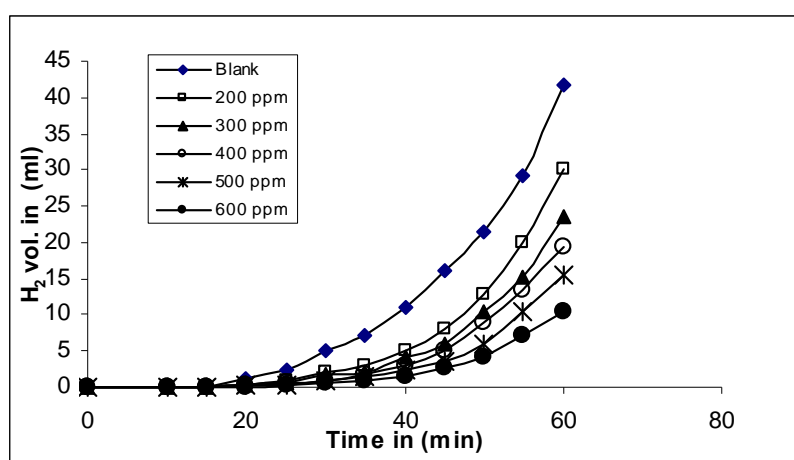
aluminate ion, $\text{Al}(\text{OH})_4^-$ that goes in solution leaving a bare surface site (ss) ready for another dissolution process (Eq. (4)) (Al-kharafi et al.,1998) Compared with the reduction of water, the reduction of oxygen can be neglected Macdonald et al.,1988). The corrosion process of Al in alkaline solution is usually considered as (Odoemelam et al,2009 ;Doche et al.1999 ;Free,2004):



As H_2 evolves (Eq. (6)), the local pH on bare surface site increases This accelerates the corrosion reaction on them, and makes it easier for the passive film to be damaged.

The free corrosion of aluminium in 2 M NaOH was characterized by rapid effervescence resulting from hydrogen gas evolution and corrosion rates in the absence and the presence of OME was studied using hydrogen evolution measurements. Figure (2) shows the variation of volume of hydrogen evolved with time for aluminium in different concentrations of NaOH without OME at 30

°C. Inspection of figure (2) shows that the hydrogen evolution starts after a certain time from the immersion of the aluminium coupon in the test solution. It may be expected that this time corresponded to the period needed by the base to destroy the pre-immersion oxide film and is known as incubation period. From figure (2), it could further be



Figure(2): Hydrogen evolution during aluminium corrosion in 2M NaOH at 30 °C in absence and presence of OME

seen that the volume of hydrogen evolved during the corrosion reaction of aluminium in 2 M NaOH containing different concentrations of OME measured as a function of reaction time at 30 °C. The plots in figure(2) illustrate the decreased deflection of hydrogen gas evolution rate on introduction of OME into the corrodent, indicating that OME actually affords corrosion inhibition of aluminium in the base environments when compared to the blank.

Similar trend was observed at 55 °C Figure (3). Further reduction in the volume of H₂ was also observed on the addition of the halide ions I⁻, Br⁻ and Cl⁻ at 30 °C (Figure(4)). Similar trend was observed at 55 °C Figure(5), but with higher values. The rates of H₂ gas evolution were observed to decrease with increasing deflection concentration, suggesting that the inhibiting action was concentration dependent. The volume of H₂ evolved at 55°C was higher than at 30 °C.

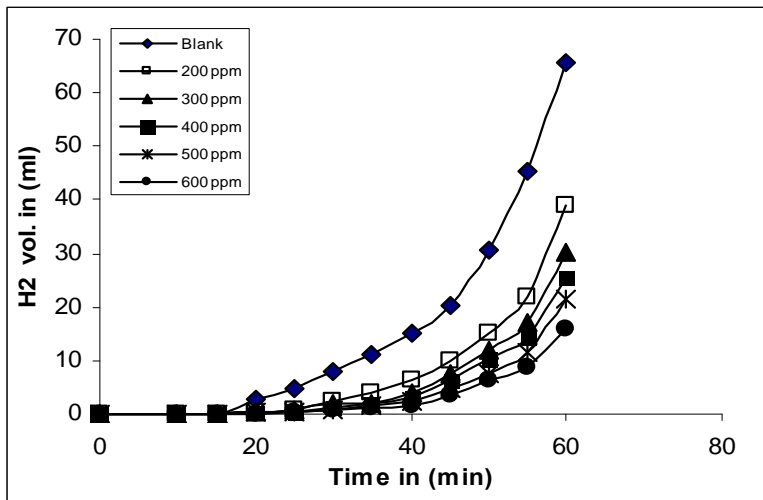


Figure (3): Hydrogen evolution during aluminium corrosion in 2M NaOH at 55 °C in absence and presence of OME

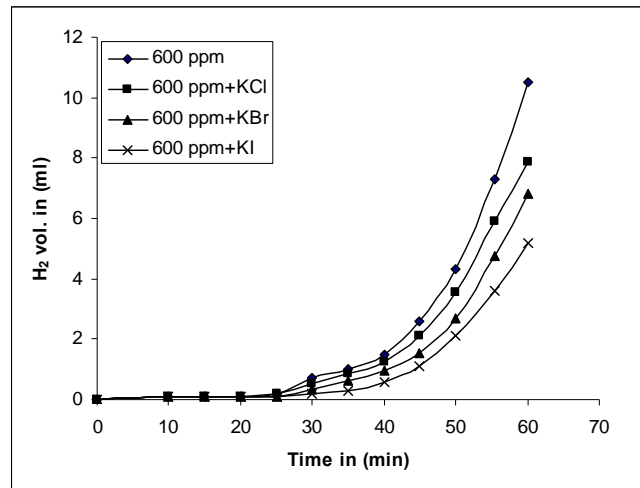
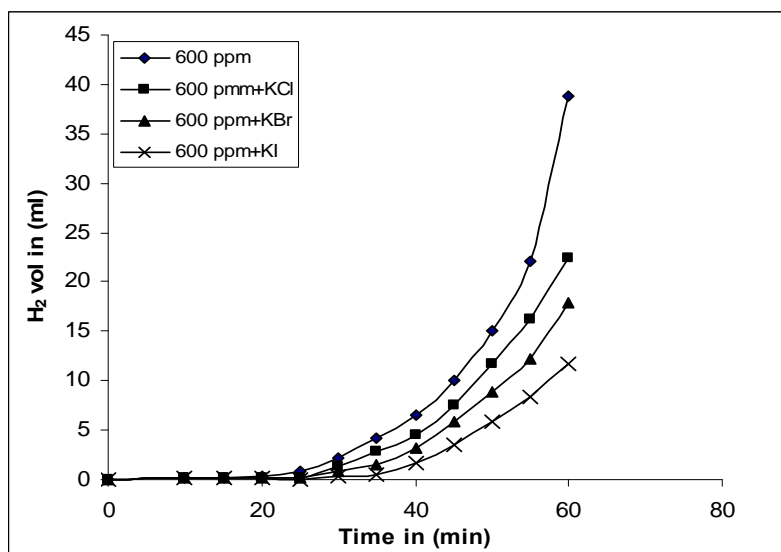


Figure (4) : Influence of halide additives on the inhibitive effect of OME during aluminium corrosion in 2M KOH at 30 °C.



Figure(5) : Influence of halide additives on the inhibitive effect of OME during aluminium corrosion in 2M KOH at 55 °C.

Visual observations showed that the hydrogen evolution decreases (i.e., the corrosion-inhibiting effect increases) upon the addition of the OME. Thus, the corrosion rate of Al decreased with the increase of the OME concentration Table (2) this trend may result from the fact that adsorption amount and the coverage of the H₂ gas evolution on the Al surface increases with increasing concentration. Thus, the Al surface is efficiently separated from the medium. The corrosion rate CR_H was determined from:

$$CR_H = \frac{V_t - V_i}{t_t - t_i}$$

where V_t and V_i are the volumes of hydrogen evolved at time t_t and t_i, respectively.

From Table (2), it is clearly seen that the corrosion rate of Al in NaOH decreased with addition of OME compared to the blank. Further reduction of corrosion rate was observed with OME in combination with halides ions as follow I⁻ < Br⁻ < Cl⁻. Also, the corrosion rate decreased with increase in the concentration of the inhibitor. This is an indication that OME showed a significant inhibitive effect on Al corrosion in the acidic environment.

Table (2): Inhibition efficiency (%I) and the degree of surface coverage (θ) of aluminum in 2M NaOH in the absence and the presence of OME and Halide AT 30 and 55 °C

System	Corrosion rate (H ₂ gas vol. ml s ⁻¹)		Inhibition efficiency (%I) (degree of surface coverage)	
	30 ° C	55 ° C	30 ° C	55 ° C
Blank	0.69	0.77	-	-
5x10 ⁻³ M KI	0.43	0.55	38.51(0.385)	43.22(0.432)
5x10 ⁻³ M KBr	0.37	0.51	30.1(0.301)	38.21(0.382)
5x10 ⁻³ M KCl	0.31	0.43	22.4(0.224)	29.42(0.29.4)
200 ppm IHIN	0.5	0.6	27.88(0.279)	22.41(0.224)
300 ppm IHIN	0.39	0.5	43.75(0.438)	34.91(0.349)
400 ppm IHIN	0.32	0.43	53.13(0.531)	44.82(0.448)
500 ppm IHIN	0.26	0.36	62.74(0.627)	53.66(0.537)
600 ppm IHIN	0.18	0.27	74.76(.748)	65.52(0.655)
600 ppm IHIN+ KI	0.086	0.19	87.5(0.875)	74.68(0.749)
600 ppm IHIN+ KBr	0.11	0.3	83.65(0.837)	61.42(0.614)
600 ppm IHIN+ KCl	0.13	0.38	81.08(0.811)	51.59(0.516)

b) Inhibition efficiency and adsorption considerations

The protective action of organic substances during metal corrosion is based on the adsorption ability of their molecules, where the resulting adsorption film isolates the metal surface from the corrosive medium. Consequently, in inhibited solutions, the corrosion rate is indicative of the number of free corrosion sites remaining after some sites have been effectively blocked by inhibitor adsorption. If it is assumed that the corrosion occurs only at the free sites such that the covered sites have a negligible corrosion rate by inhibitor, and based on gasometric measurements, the values of inhibition efficiency (%I) for various concentrations of OME after 1 h of immersion at 30 and 55 °C are given in Table (2). The relation equation determines the inhibition efficiency (% I): and hence the degree of surface coverage (θ) can be calculated as follows (Odoemelam et al, 2009):

$$\%I = \left[1 - \frac{V_{H_t}^1}{V_{H_t}^o} \right] \times 100$$

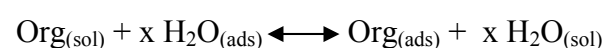
$$\theta = \left[1 - \frac{V_{H_t}^1}{V_{H_t}^o} \right]$$

where $V_{H_t}^1$ is the volume of hydrogen evolved at time "t" for inhibited solution and $V_{H_t}^o$ that for an uninhibited solution.

Table (2) illustrates the variation of inhibition efficiency with concentration for the studied OME. The table indicates that % I increased

with concentration of the OME but decreased with increase in temperature. This is attributed to the decrease in the protective nature of the inhibitive film formed on the metal surface (or desorption of the inhibitor molecules from the metal surface) at higher temperatures (Doche et al. 1999). This suggests a physical adsorption mechanism. Physical (electrostatic) adsorption takes place when inhibition efficiency decreases with increase in temperature (whereas chemical adsorption takes place when inhibition efficiency increases with increase in temperature (Free, 2004)). The inhibitive action of the inhibitor is due mainly to the presence of hetero atoms such as oxygen, nitrogen and aromatic rings with π -bonds in the OME molecules, which serve as centers of adsorption onto the metal surface. Also the inhibition efficiency effect increases in order $Cl^- < Br^- < I^-$, which seem to indicate that the radii of halide ions may have an important role to play.

The adsorption of organic adsorbate on a metal surface is regarded as a substitutional adsorption process between the organic molecule in the aqueous solution ($Org_{(sol)}$), and water molecules adsorbed on the metallic surface ($H_2O_{(ads)}$) (Umoren et al., 2008):



Where x is the size ratio representing the number of water molecules replaced by one molecule of organic adsorbate.

The adsorption of inhibitor compounds can be described by two main types of interaction : physical and chemisorptions. This influenced by the nature and charge of metal, the chemical structure of the inhibitor and the type of electrolyte.

The values of the degree of surface coverage area θ were evaluated at different concentration of the OME (Table (2)) in 2M NaOH solution .Attempts were made to fit θ values to various adsorption isotherms. The Temkin adsorption isotherm fit the experimental data using the following equation (Okafor et al., 2009)Shengtao et al.,2009) :

$$\exp(-2f\theta) = k_{ads}C$$

where k_{ads} , C and f represent the equilibrium constant of adsorption process and additive concentration and molecules interaction parameter ,respectively . A plot of θ against

$\ln C$ would give a straight line of intercept $\ln k$. The plot shown in figure (6) suggested that the Temkin adsorption isotherm is obeyed. Table (3) demonstrate the calculated values of equilibrium constant and standard free energy of adsorption (Xueming, 2007):

$$k = \frac{1}{55} \exp\left[\frac{-\Delta G^0_{ads}}{RT}\right]$$

where R is the gas constant .the value 55.5 is the concentration of water in the solution in mol/l.

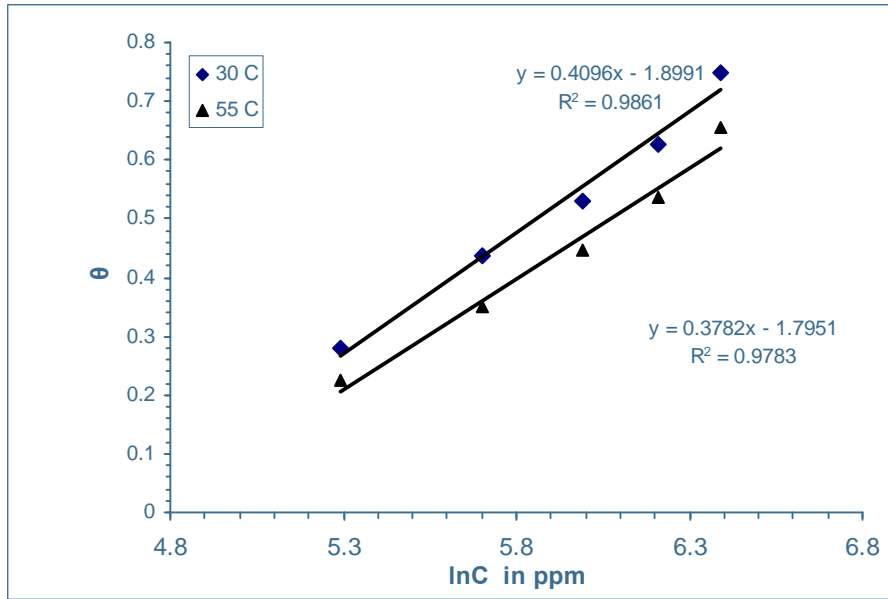
the negative value of f indicates that the repulsion exists at neighboring adsorption sites in the adsorption layer (Umoren et al.,2008), also K_{ads} denotes the strength between the adsorbate and adsorbent .Small values of K_{ads} imply restricted efficiency adsorption. K_{ads} values are seen to decrease with temperature increase suggesting that the inhibitors are physically adsorbed onto aluminum surface.

Table (3): Thermodynamic parameter for adsorption of OME on the Al 6063 in 2M NaOH at 30 and 55 °C

Temperature in (°C)	K_{ads} (M^{-1})	ΔG^0_{ads}	f	R^2
30	1.141	-10.45	-1.1	0.9816
55	1.05	-11.086	-1.315	0.978

Generally values of ΔG^0_{ads} until -20 kJmol^{-1} are consistent with the electrostatic interaction between the charge molecules and the charge of metal surface (physical adsorption)

(Scendo,2008;Donahue et al.,1965). The values of standard free energy Table (3) suggest physical adsorption of OME on aluminum 6063 surface.



Figure(6): Temkin isotherm adsorption of OME in the surface of Al 6063 in 2M NaOH at 30 and 55 °C

c) Effects of temperature

Temperature has a great effect on the rate of metal electrochemical corrosion. In case of corrosion in a neutral solution (oxygen depolarization) the increase in temperature has a favorable effect on the over potential of oxygen depolarization and the rate of oxygen diffusion but it leads to a decrease of oxygen solubility. In case of corrosion in an base medium (hydrogen depolarization), the corrosion rate increases exponentially with temperature increase because the hydrogen evolution over potential decreases (Mohammed et al.,2009). An experimental dependence of an integrated Arrhenius-type equation is observed between the corrosion rate and temperature (Zaharieva et al.,2009):

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

where ρ_2 and ρ_1 are the corrosion rates at temperature T_1 and T_2 , respectively, and R the molar gas constant. An estimate of heat of adsorption was obtained from the trend of surface coverage with temperature as follows (Zaharieva et al.,2009):

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

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. Some studies (Lowmunkhong et al.,2010 ;Umoren et al.,2008) showed that compared with the activation energy, **Ea** in the absence of inhibitors, higher values of **Ea** were found in the presence of inhibitors. Other studies (Mohammed et al.,2009 ;Zaharieva et al.,2009) showed that in the presence of inhibitor the activation energy E_a was lower than that in the absence of inhibitor. In the

present study, however, it could be found that the values of E_a in the presence of different concentrations of OME were higher than that

in its absence. This is often interpreted as an indication of the

Table (4): Calculated value of activation energy, heat adsorption for aluminum corrosion in 2 M NaOH with inhibitor OME and inhibitor +halide mixture .

Conc. Of OME in ppm	E_a (kJ mol ⁻¹)	Q_a (kJ mol ⁻¹)
Blank	3.608	-
200	6.0208	-96.888
300	8.4261	-12.284
400	21.647	11.005
500	10.816	-12.382
600	13.914	-14.661
600+ 0.05 M KI	34.561	-27.486
600+ 0.05 M KBr	31.919	-38.496
600+ 0.05 M KCl	26.94	-45.99

formation of an adsorptive film of a physical electrostatic character (Obot et al., 2008). Thus, the adsorbed OME molecules create a physical barrier to charge and mass transfer (Ezuber et al., 2008). The negative Q_{ads} values also signify that the degree of surface coverage decreased with rise in temperature. The reason for this, as suggested by (Oguzie ,2007), may be that the attainment of physical adsorption equilibrium is usually rapid and the process readily reversible whereas in chemisorptions, the occurrence of chemical reactions at the metal surface makes the process relatively slow and not readily reversible.

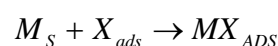
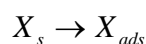
d) Synergism consideration

The synergism parameter S_1 was evaluated using the relationship below, initially given by Aramaki and Hackermann and reported elsewhere (U Moran ,2009):

$$S_1 = \frac{1 - I_{1+2}}{1 - I'_{1+2}}$$

where $I_{1+2} = I_1 + I_2$, I_1 = inhibition efficiency of iodide ion, I_2 = inhibition efficiency of OME, and I'_{1+2} is measured inhibition efficiency for OME in combination with halide ions. The calculated values of synergism parameters for the various concentrations of OME are presented in table (5). The value of S_1 greater than unity is an indication that the enhanced inhibition efficiency resulting from the addition of Halides ion to OME is synergistic in nature.

This can be explained on the basis that Γ^- , Br^- and Cl^- ions has a greater tendency to be adsorbed on the surface of and this may be responsible for the synergistic effect of halides ion on OME. Halide ions are normally strongly adsorbed on metal surfaces where the chemisorbed ions enter the metallic part of the charged of the metal surface (Umoren et al., 2009). Thus the inhibitor is not adsorbed directly on the metal surface itself, but rather by coulombic attraction to the adsorbed halide ions on the metal surface. This process is similar to the so-called phenomenon of anion induced adsorption and may be represented by the highly simplified mechanism (Ebson ,2003 ; Li et al.,2006):



where X_s and M_s designate the halide ion and organic species, respectively, in the bulk state, X_{ads} and MX_{ads} refer to halide and ion pair, respectively, in the adsorbed state. This ion pair interaction consequently increases the surface coverage thereby reducing metal dissolution.

S_1 approaches 1 when no interaction between the inhibitor compounds exists, while $S_1 > 1$ points to a synergistic effect. In the case $S_1 < 1$, the antagonistic interaction prevails, which may be attributed to competitive adsorption.

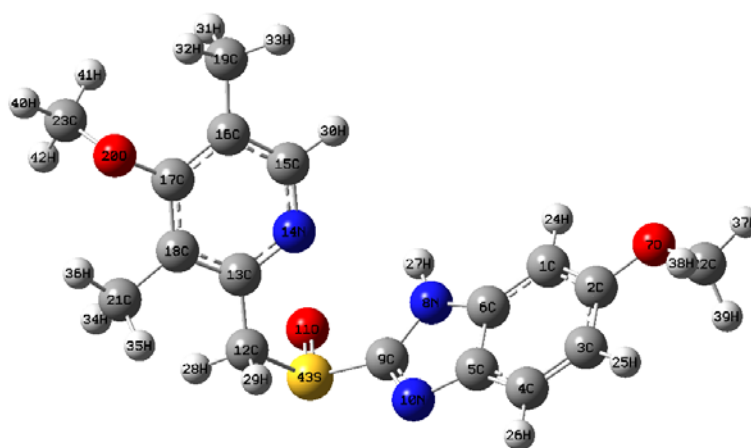
Table (5) : Synergistic parameters (S_1).

System	S_1	
	30°C	55°C
KI +600 ppm of OME	1.29	1.829
KBr+600 ppm of OME	1.257	1.7
KCl +600 ppm of OME	1.2	1.86

e) Theoretical calculations

The researchers are often encouraged to use theoretical data in their studies not only to support their experimental results and but also to find the efficient way to minimize the chemical expenditures. Therefore , recently more corrosion publications contain substantial

quantum chemical calculations (Hasanov et al.,2010). Accordingly, quantum chemical calculations are performed to investigate the structural parameters affect the inhibition efficiency of inhibitors .Geometric and electronic structures Figure(7) and table (6) of the inhibitors are calculated by the optimization of their bond lengths, bond angles and dihedral



Figure(7): Optimized geometry of OME using AM1

angles. The optimized molecular structures with minimum energies Mulliken charge distributions obtained from the calculations are given in figure(7) which show that (OME) are non planer molecules with no center of symmetry . The surface coverage therefore cannot be uniform as is observed for planer molecules. The shape also suggests that for form a passive/resistive layer these molecules

can be better oriented at lower concentration only. At higher concentrations ,there will be considerable steric hindrance and gaps because of which passivity will tend to be destroyed .Due to the non planer shape of these inhibitors ,it dose not act as a perfect donor of electrons, and this may cause the cracks in protective covering layer (Cruz et al.,2001).

Table (6): Some geometrical parameter for OME

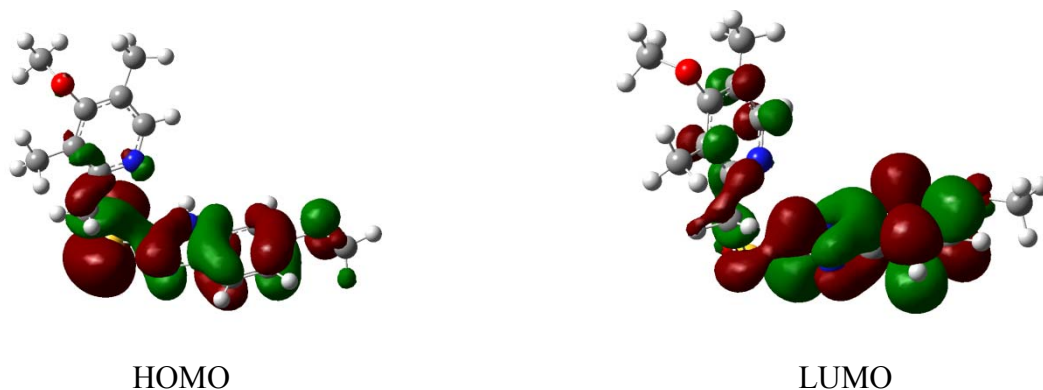
Atoms	C9-S43	S43-C12	C12-C13	C9-N8	C9-N10	C9-N14
Bond length	1.728	1.757	1.491	1.409	1.352	1.352
Dihedral	C9S43C12C13	N10C9S43C12	N8C9S43C12	S43C12C13N14		
	66.747	77.914	-105.782	-19.328		
angel	C9S43C12	C12C13N14	N8C9S43	N10C9S43	C12C1C18	
	102.380	118.255	124.113	123.391	118.983	

According to the frontier molecular orbital theory, the formation of a transition state is due to an interaction between frontier orbitals (HOMO and LUMO) of reacting species

Wang et al., 2009). E_{HOMO} is often associated with the electron donating ability of a molecule. Several researches have shown that the adsorption of an inhibitor on the metal

surface can occur on the basis of donor–acceptor interactions between the p-electrons of the heterocyclic compound and the vacant d-orbital of the metal surface atoms (Obot et al 2009). High E_{HOMO} values indicate that the

molecule has a tendency to donate electrons to appropriate acceptor molecules with low energy empty molecular orbital. Increasing values of the E_{HOMO} facilitate



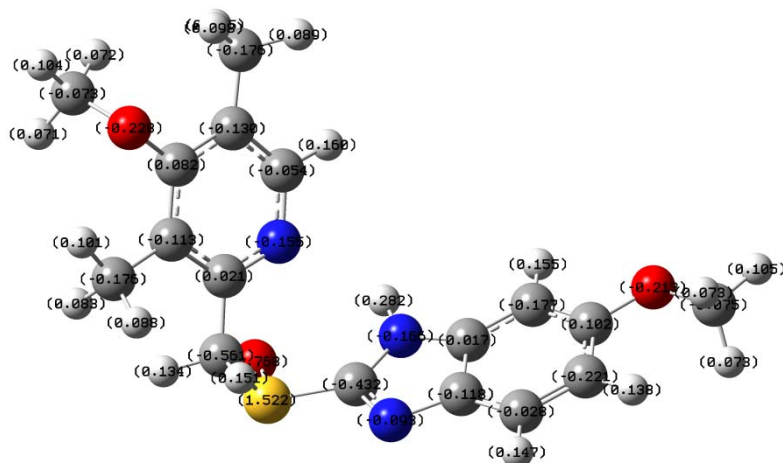
Figure(8). Three dimensions pictures of frontier orbital density distribution HOMO and LUMO

adsorption (and therefore inhibition) by influencing the transport process through the adsorbed layer. E_{LUMO} indicates the ability of the molecules to accept electrons. The lower values of E_{LUMO} , the more probable it is that the molecule would accept electrons. Low absolute values of the energy band gap (ΔE) give good inhibition efficiencies, because the energy to remove an electron from the last occupied orbital will be low.

The calculated theoretical parameters for OME are [E_{HOMO} (-8.534) , E_{LUMO} (-0.278 eV) and ΔE (8.254 eV). The lowest E_{LUMO} and energy gap the better inhibition efficiency is still valid in our study.

The dipole moment of (OME) is 2.351 is another indicator of the electronic distribution in a molecule and is one of the properties used to discuss and to rationalize the structure (Obot et al 2010). Although, there is a lack of agreement in the literature on the correlation between the dipole moment and inhibition efficiency (Arslan et al., 2009) .

The use of Mulliken population analyses to probe the adsorption centres of inhibitors have been widely reported [Li et al.,2009;Issa et al.,2008 ; Kandemirli et al.,2007). Figure (9) explained the Mulliken distribution of charge on the OME inhibitor.



Figure(9): Mulliken charge for atoms of OME using AM1.

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دراسة خواص تثبيط الاومبرازول على تأكل الألمنيوم 6063 في الوسط القاعدي

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الخلاصة

تضمن البحث تقييم تأثير عقار الاومبرازول على تأكل سبيكة الامنيوم 6063 في وسط قاعدي من 2 مولاري من هيدروكسيد الصوديوم باستخدام طريقة تحرير الهيدروجين عند درجة حرارة 30 و 55 مئوي . دلت النتائج ان الاومبرازول ذو فعل تثبيطي جيد و ان كفاءة التثبيط تزداد مع زيادة تركيزه كما بينت الدراسة ان كفاءة التثبيط تزداد مع زيادة درجة الحرارة من 30 الى 55 مئوي في حالة وجود المثبط و الهاليدات او عدم وجودهم. تم حساب قيم طاقة التنشيط المرافقة لعملية الامتزاز و حرارة الامتزاز و التغير في الطاقة الحرة للامتزاز حيث دلت الأخيرة على حدوث امتزاز فيزيائي تلقائي، وان المثبط يخضع لعلاقة Temkin للامتزاز الايزوثيرمي. كما درس أيضا التأثير المتبادل التعاوني (Synergism parameter (S_1) بين كل من (ايون الكلور و البروم و اليود) و المثبط تحت الدراسة ، أظهرت النتائج ان الزيادة في كفاءة التثبيط كان بسبب إضافة الهاليدات كنتيجة للتأثير المتبادل التعاوني (Synergism). حسبت أيضا بعض مقاييس الميكانيك الكيميائي و توزيع موليكن للشحنة باستخدام طريقة AMI الشبه تجريبية بغية فهم أكثر لميكانيكية تثبيط عملية التآكل. دراسة خواص تثبيط الاومبرازول على تأكل الألمنيوم 6063

في الوسط القاعدي