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# Experimental and Quantum Chemical Studies of the Inhibition of Copper with Sodium Dodecyl Sulphate (SDS) in Acidic Medium

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## Abstract

This work investigates the inhibitive properties of sodium dodecyl sulphate (SDS) on the corrosion of copper (Cu) in nitric acid using gasometric methods. The inhibition efficiency increases with time and concentration of SDS. The corrosion rate of copper decreases as concentration of SDS increases. Adsorption of the SDS on the surface obeyed the Langmuir adsorption isotherm. The high negative values of the kinetic parameter B suggest that the inhibitor's effectiveness increases with temperature. The equilibrium constant and the free energy of adsorption of SDS to copper are negative and large. This observation implies that the adsorption mechanism maybe chemisorption. The quantum chemical calculation of copper dodecyl sulphate shows that the energy change in the HOMO-LUMO energy of the moiety is positive and small. This observation implies that the SDS is an efficient inhibitor. The high dipole moment obtained implies that corrosion inhibition of Cu is enhanced by adsorption of SDS and this observation correlates with the observed experimental inhibition efficiency.

## Keywords

Corrosion Inhibition, Copper, Gasometric Methods, Adsorption, Inhibition Efficiency, Sodium Dodecyl Sulphate (SDS)

## 1. Introduction

Copper exhibits excellent electrical, thermal and mechanical properties that makes it a relatively noble metal used for various applications in building construction, machinery, equipment and consumer products to mention a few [1]

[2] [3].

Corrosion is an age long problem affecting infrastructures, production, and transportation in the industrial sector. Various organic compounds and natural inhibitors are proven methods of preventing and controlling corrosion of metals. The choice of corrosion inhibitors depend on cost, toxicity, availability and biodegradability of the substance because of the environment [4]-[13]. It has also been reported that inhibitors reduce corrosion rate through modification of corrosion potential, retardation of cathodic and anodic corrosion reactions via polarization and passivation of the metal surface, and by adsorption to the metal surface [14] [15] [16]. Copper is corrosion resistant in water but corrodes easily in acid and alkaline solutions. Various researches have shown that the passivation layer built in copper is from simple $Cu_2O$ or a duplex of $Cu_2O/CuO{\cdot}Cu(OH)_2$ structure and it depends on the pH of solution and the electrode potential [14] [15].

Hayon *et al*. [1] have studied corrosion of Copper in borate solutions and observed using electrochemical DC at pH 7.5 that there is no passivity breakdown of copper in the presence of SDS. They have also shown that dodecyl sulphate ions accelerate anodic dissolution of copper metal to $Cu^{2+}$, at low pH. They attributed the breakdown in passivity in the presence of SDS to the formation of $Cu(DS)_2$ complex. Studies have shown that SDS acts as inhibitor for corrosion of metals like nickel, aluminium, steel, in chloride medium and mild steel, stainless steel and also copper in acidic medium [16] [17]. Sodium dodecyl sulphate is a surfactant whose presence even at very low concentrations in any medium provides desirable properties useful to many processes in petrochemical, food, paint, detergent and coating industries. The adsorption of surfactants on metal surfaces is extremely important in corrosion inhibition and metallic electro deposition. The surface of the surfactants on electrodes have been shown to have significant effects on the kinetics of electron transfer at electrodes including surface blocking, and electrostatic interactions between solutes and adsorbed surfactants. Mobin *et al*. and Igua *et al*. suggested that the interaction between surfactants and the metal surface is related to the structure of the absorbed species [17] [18]. It has been reported that corrosion inhibition of surfactants is related to its ability to aggregate at interfaces and in solution and corrosion inhibition by surfactant depends on its concentration [19] [20].

The current trend of correlating experimental and quantum chemical studies of inhibitors and the successful application of density functional theory have kindled much interest in studying the inhibitor efficiency of sodium dodecyl sulphate (SDS) on copper in acidic medium. Quantum chemical studies have been deployed to relate the molecular properties of different organic compounds their inhibition efficiencies [21]-[27]. The molecular and electronic parameters obtained from these calculations include the energy gap obtained from the highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital LUMO. The difference in the energy for the HOMO-LUMO transition is an

indicator of the efficiency of the inhibitor been studied [22] [23] [24] [25].

This study investigates the molecular properties using the density functional theory (DFT) of the inhibitor efficiency of sodium dodecyl sulphate (SDS) an anionic surfactant on the corrosion of copper in nitric acid solution. The hardness and the tensile strength of copper metal in the with and without sodium dodecyl sulphate are analyzed.

## 2. Materials and Methods

Copper (99.9%) and Sodium dodecyl sulphate (SDS) molecular formula $C_{12}H_{25}NaO_4S$ was purchased from Fessy electrical company Ibadan, Nigeria and Surechem Ltd. England respectively. Nitric acid ($HNO_3$) was obtained from Aldrich Chemical and Co. The copper sheet was mechanically pressed cut into different coupons of dimension 2 cm by 2 cm by 0.3 cm. Each coupon was polished and drilled at one end, degreased in acetone, dried and preserved in air tight desiccator at room temperature. The stock solution of 1M SDS was prepared in 10 mL $HNO_3$ from which working concentrations of 2.75 mM, 3.5 mM, 7.0 mM and 10mM were prepared by simple dilution. Corrosion studies were carried out using gasometric method. This method involves measuring the volume of gas evolved when a metal reacts with an acid from the cathodic reaction of the corrosion process and this is proportional to the rate of corrosion [28]. 100 mL of the corrodent (2M $HNO_3$) was poured into the two necked flask, the initial volume of air in the graduated burette was noted, and the Copper coupon of approximately 4 g was immersed into the corrodent, the flask was quickly closed and the volume of $H_2$ gas evolved from reaction was monitored by volume change in the graduated burette at different time intervals of about 3 hours. Measurements were carried out in duplicate.

The corrosion of copper in 2M $HNO_3$ was characterized by rapid evolution of $H_2$ gas. The rate was also calculated with and without sodium dodecyl sulphate (SDS) using the Equation (1)

$$C_{RH} = \frac{V_t - V_i}{t_t - t_i} \tag{1}$$

where $V_t$ and $V_i$ are volumes of $H_2$ evolved at time $t_t$ and $t_i$ respectively, $C_{RH}$ is the corrosion rate. The inhibition efficiency was also calculated using:

The rate of evolution of gas ($RV$) is obtained from the slope of the graph plotted for volume of gas evolved against time.

$$RV = \frac{\Delta V}{\Delta T} \tag{2}$$

$$\%I = \frac{RV_{blank} - RV_{inh}}{RV_{blank}} \tag{3}$$

Inhibitor surface area of coverage $\theta$ is calculated from the expression

$$\theta = \frac{\%I}{100} \tag{4}$$

where $RV_{blank}$ and $RV_{inh}$ are the rate of evolution of gas with and without SDS respectively, $\%I$ is the percentage inhibition efficiency.

### Computational Studies

Quantum chemical calculations using density functional theory (DFT) were simulated using "SPARTAN" 10 nI software [29]. The calculated parameters include the highest occupied molecular orbital (HOMO), the lowest occupied molecular orbital (LUMO), dipole moment ($\mu$), ionization potential ($I$), electron affinity ($A$), absolute electronegativity ($\chi$), absolute hardness ($\eta$), global softness ($\sigma$) and electrophilicity index ($\omega$) were obtained from the optimized molecular structure.

Using the Koopmans theorem, [30];

Ionization potential "$I$" $= -E_{\text{HOMO}}$;

Electron affinity "$A$" $= -E_{\text{LUMO}}$.

The absolute hardness $\eta$ and global softness σ were calculated [31] as follows,

Absolute hardness "$\eta$" $= \dfrac{E_{\text{HOMO}} - E_{\text{LUMO}}}{2}$.

Global softness "$\sigma$" $= \dfrac{1}{\eta}$.

Electrophilicity index "$\omega$" $= \dfrac{\chi}{2\eta}$.

## 3. Result and Discussion

### 3.1. Gasometric Measurement

The corrosion of copper in 2M $HNO_3$ in the with and without Sodium dodecyl sulphate has been studied at 30˚C using gasometric methods. Table 1 shows the inhibition efficiency and the rate of evolution of gas at different concentrations of SDS.

The Inhibition efficiency (I.E) increases as the concentration of Sodium dodecyl sulphate (SDS) increases with a maximum I.E of 52.03% at 0.30 g/L of SDS. The rate of evolution of gas deceases as SDS concentration and inhibition efficiency increases. This implies that more SDS molecules were adsorbed on the

Table 1. Percentage inhibition efficiency of sodium dodecyl sulphate at different concentrations at 30˚C.

| SDS concentration (g/L) | Rate of evolution of gas (RV) | Surface coverage of adsorption ($\theta$) | Inhibition efficiency (%) |
|---|---|---|---|
| 0.05 | 0.186 | 0.3137 | 31.37 |
| 0.10 | 0.183 | 0.3247 | 32.47 |
| 0.15 | 0.179 | 0.3395 | 33.95 |
| 0.20 | 0.153 | 0.4354 | 43.54 |
| 0.25 | 0.145 | 0.4649 | 46.95 |
| 0.30 | 0.130 | 0.5203 | 52.03 |

surface of copper forming a protective layer that inhibits its corrosion (Table 1, Figure 1).

### 3.2. Kinetic and Thermodynamic Treatment of Gas Evolution Result

Assuming that the plot of corrosion rate ($CR$) of copper in the presence of SDS against concentration of inhibitor-SDS (Figure 2) obeys the kinetic relationship in Equation (5)

$$\log CR = \log k + B \log C \tag{5}$$

And B obtained from the slope in Figure 2 is defined as the reaction constant which measures the effectiveness of the inhibitor while k is the rate constant of the reaction. [4] [32] [33] [34] [35]

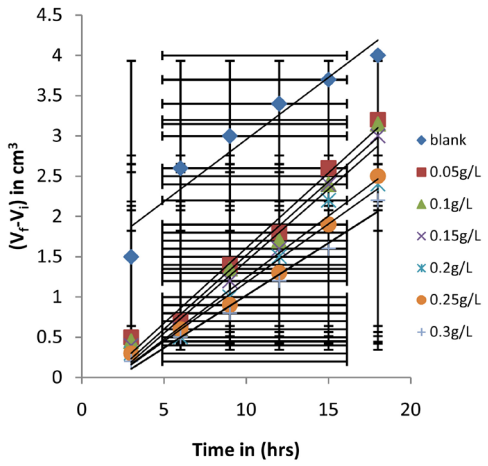



Figure 1. Volume of gas evolved versus time of copper in 2M $HNO_3$ with and without of SDS at 30˚C.

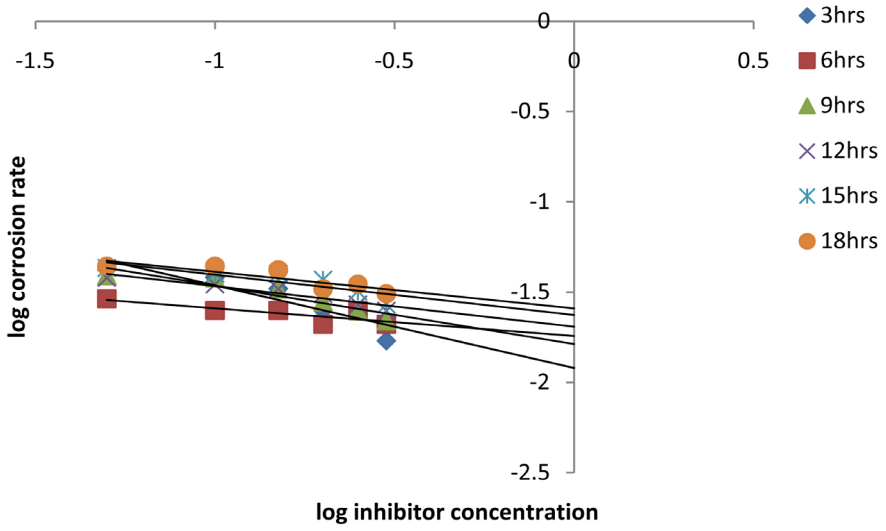



Figure 2. Variation of log corrosion rate log concentration of SDS for corrosion of copper in 2M $HNO_3$ at 30˚C.

The values of B obtained for this experiment are negative (Table 2). This implies that the rate of corrosion is inversely proportional to the concentrations of SDS. SDS becomes more effective as its concentration increases. The negative value of B decreases in magnitude as the time increases which implies that SDS effectiveness will increase with temperature.

The rate constant *k*, defined as the corrosion rate at the inhibitor concentration of unity increases with time as expected of a first order kinetics. The adsorption isotherm fitted the Langmuir model (Figure 3) and the equilibrium constant for adsorption $K_{ads}$ obtained from Equation (6).

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \tag{6}$$

where $C_{inh}$ is the concentration of inhibitor and $\theta$ is the degree of surface coverage.

The free energy of adsorption $\Delta G_{ads}$ obtained from Equation (7). The enthalpy

Table 2. Kinetic parameters for corrosion inhibition of copper in the presence of SDS at 30˚C.

| Time of immersion (hours) | *B* | log*k* | $k \times 10^{-2}$ ($hr^{-1}$) |
|---|---|---|---|
| 3 | −0.4580 | −1.9198 | 1.2028 |
| 6 | −0.1524 | −1.7423 | 1.8101 |
| 9 | −0.3244 | −1.7881 | 1.6289 |
| 12 | −0.2244 | −1.6912 | 2.0361 |
| 15 | −0.2231 | −1.6269 | 2.3610 |
| 18 | −0.2024 | −1.5896 | 2.5728 |

Table 3. Thermodynamic parameters for inhibition of corrosion of copper in the presence of SDS at 30˚C.

| $K_{ads}$ | $\Delta G_{ads}$ kJ/mol | $\Delta H_{ads}$ kJ/mol | $\Delta S_{ads}$ J/mol/K |
|---|---|---|---|
| 7.4349 | −75.0556 | −5.0538 | 231.0290 |

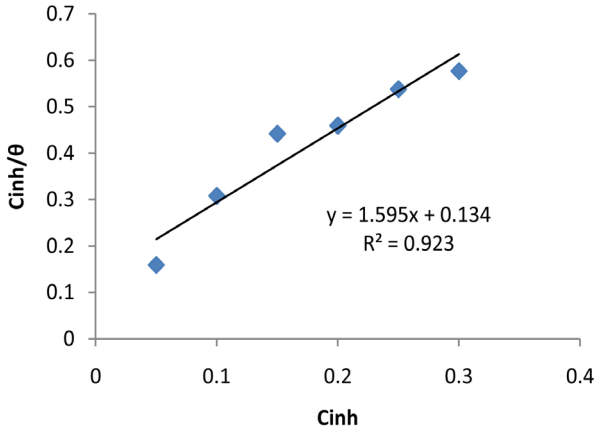



Figure 3. Langmuir adsorption isotherm for the corrosion inhibition of copper with SDS at 30˚C.

$\Delta H_{ads}$ for the process obtained from van't Hoff Equation (8) and the entropy $\Delta S_{ads}$ from the Gibbs Equation (9) is shown in **Table 3**.

$$\ln K_{ads} = \ln\left(55^{-1}\right) - \Delta G_{ads}\left(RT^{-1}\right) \tag{7}$$

$$\ln K_{ads} = \frac{-\Delta H_{ads}}{RT} + C \tag{8}$$

$$\Delta G_{ads} = \Delta H_{ads} + T\Delta S_{ads} \tag{9}$$

The value of $K_{ads}$ for this experiment is positive and small and $G_{ads}$ is negative and large (~−75.06 kJ/mol). The negative value of $\Delta G_{ads}$ shows that the reaction is spontaneous. The negative large value of $\Delta G_{ads}$ obtained in his experiment is consistent with charge transfer or sharing from the sodium dodecyl sulphate (SDS) to the metal surface to form a coordinate bond between the metal and inhibitor which implies the mechanism of adsorption is chemisorption. Generally negative values of the magnitude −40 kJ/mol or more signify chemisorptions [7] [12]. The negative value of $\Delta H_{ads}$ implies that adsorption process is exothermic.The entropy of adsorption $\Delta S_{ads}$ is 231.0290 J/mol/K is positive. This observation indicates that the adsorption of SDS on copper shows an ordered system.

### 3.3. Quantum Chemical Treatment of Data

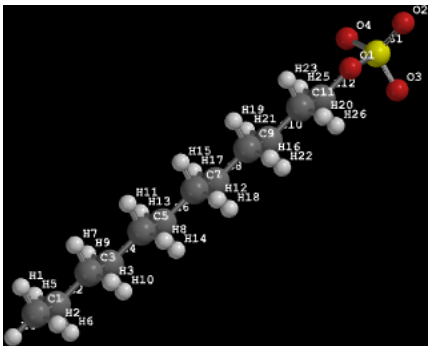
Quantum chemical calculations using density function theory (DFT were simulated using Spartan 10 software. The properties calculated were obtained after geometric optimization of the structures as shown in **Figures 4(a)-(c)**. and the calculated quantum chemical parameters obtained in this study tabulated as 4.

"*The frontier orbital molecular theory of chemical reactivity shows that transition of electron is due to interaction between highest occupied molecular orbital* (*HOMO*) *and the lowest unoccupied molecular orbital* (*LUMO*) *of reacting species*" [24] [36].

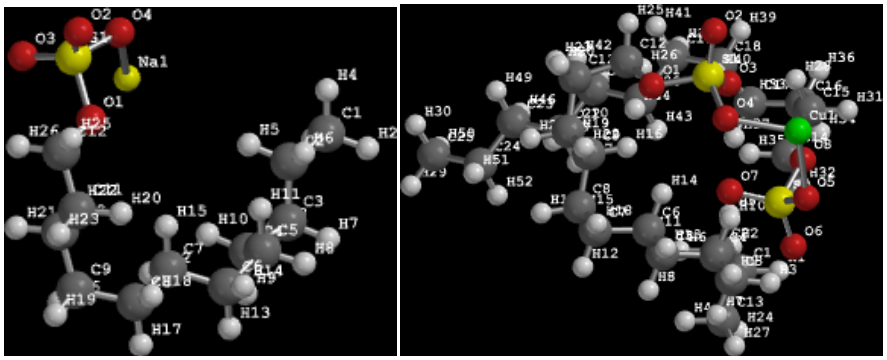
The quantum mechanical parameter which represents the ionization potential and the ability of a molecule to donate electron to an acceptor with an empty molecular orbital of lower energy is $E_{\text{HOMO}}$ [37]. The inhibitor SDS $E_{\text{HOMO}}$ obtained is −9. 97eV and that of copper dodecyl sulphate (CDS) is −9.43 eV implies that SDS donates electrons to the unoccupied d orbital of $CU^{2+}$ ion and also accepts electrons from the metal ion to form a feedback bond (**Figure 4(c)**).

The ease of forming a feedback bond depends on the value of $E_{\text{LUMO}}$. The lower the $E_{\text{LUMO}}$ the easier it is for the inhibitor to accept electrons from the *d* orbital of the metal [38] [39]. The $E_{\text{LUMO}}$ observed for this experiment is −1.27 eV which implies that the inhibitor SDS will accept electrons from the d orbital of copper metal.

The band gap energy $\Delta E$ is a function of adsorption of inhibitor on the surface of a metal, a decrease in $\Delta E$ implies an increase in reactivity and inhibition efficiency of the molecule. The calculated $\Delta E$ value for this study is 8.7 eV which implies the highest inhibition efficiency and reactivity are in agreement with experimental observations.



(a)



(b) (c)

**Figure 4.** (a) Optimized structure of Dodecylsulphate (DS); (b) Optimized geometry of Sodium Dodecylsulphate (SDS); and (c) Optimized geometry of Copper Dodecyl sulphate (CDS).

**Table 4.** Computational data of corrosion of copper in the presence of sodium dodecyl sulphate obtained using SPARTAN 10 nI.

| Parameters | Dodecyl sulphate (DS) | Sodium Dodecyl sulphate (SDS) | Copper Dodecyl sulphate (CDS) |
|---|---|---|---|
| $E_{\text{LUMO}}$ (eV) | −0.58 eV | −1.27 eV | −1.31 eV |
| $E_{\text{HOMO}}$ (eV) | −11.13 eV | −9.97 eV | −9.43 eV |
| $\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$ (eV) | 10.55 eV | 8.7 eV | 8.12 eV |
| Dipole moment, $\mu$ (Debye) | 2.48 Debye | 11.19 Debye | 3.52 Debye |
| Ionization energy, $I$ (eV) | 11.13 eV | 9.97 eV | 9.43 eV |
| Electron affinity, $A$ (eV) | 0.58 eV | 1.27 eV | 1.31 eV |
| Absolute electronegativity, $\chi$ (eV) | 5.86 eV | 5.62 eV | 5.37 eV |
| Absolute hardness, $\eta$ (eV) | 5.28 eV | 4.35 eV | 4.06 eV |
| Global softness, $\sigma$ ($eV^{-1}$) | 0.189 $eV^{-1}$ | 0.230 $eV^{-1}$ | 0.246 $eV^{-1}$ |
| Electrophilicity index, $\omega$ (eV) | 3.252 eV | 3.630 eV | 3.551 eV |
| Total energy change, $\Delta E_T$ (eV) | −1.32 eV | −1.09 eV | 1.02 eV |

The stability and the reactivity of the molecule are measured by its hardness or softness. Absolute hardness and global softness are measure of the molecular stability and reactivity of a molecule. A hard molecule has a large $\Delta E$ while a soft

molecule has small $\Delta E$ value [40]. Soft molecules donate electrons with ease and efficiently so they are more reactive than hard molecules [3]. The data obtained in this study for SDS (**Table 4**) indicates a low value for absolute hardness at 4.35 eV and high value for global softness at 0.23 eV; this implies that SDS is a soft molecule and an efficient electron donor and inhibitor. This observation is in agreement with Abdel Raham *et al*. [3].

The dipole moment $\mu$ describes the polarity of a molecule [41]. The high dipole moment observed at 11.9D for SDS will probably increase its absorption to the metal surface as earlier proposed by Kikuchi [42]. The total energy calculated by the quantum chemical method for this study is −1.09 eV is the minimum total energy which in agreement with Ju and Li [43] "is the total energy of the system in the presence of static external potential and it is a function of the charge density. The electronic charge density which gave rise to this minimum energy is the exact single particle ground state energy".

## 4. Conclusions

- Inhibition efficiency of SDS increases as the concentration of SDS increases and the rate of evolution of gas decreases as SDS concentration decreases.
- The effectiveness SDS as an inhibitor of corrosion of copper will likely increase with temperature as indicated by the value of B the reaction constant.
- The free energy of the reaction is large and negative which suggests that SDS is chemically adsorbed *i.e*. mechanism of adsorption is chemisorptions.
- Quantum chemical parameters for Cu-SDS shows a good correlation between the electronic structure of SDS and its potential as an inhibitor for the corrosion of copper.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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