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Electrochemical and molecular dynamics simulations of corrosion inhibition efficiency of N-phenylpiperazinylsulfamide on Al surface in H2SO4

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INTRODUCTION

The acidic medium is highly encountered in the industrial fields such as cleaning, descaling and pickling [1] , which caused lot of degradations so the use of inhibitors is considered as a must to minimize the extent of corrosion in the acidic solutions [2] and providing protection of metal [3].The use of inhibitors is one of the most practical methods for protection against corrosion especially in acid descaling bathes to prevent not only metal dissolution but also acid consumption by reducing the rate of either or both partial reactions of the corrosion process. The studies of organic and eco-friendly corrosion inhibitors are of g reat interest from an environmental perspective and are attracting a significant level of attention [4]. and to mitigate these effects the use of organic inhibitors seems to be an efficient and suitable option because it have a promising future for the quality of the environment because they do not contain heavy metals or other toxic compounds. Extracts from leaves, seeds, fruits and roots contain compounds with nitrogen, sulfur and oxygen described as efficient corrosion inhibitors indifferent to the aggressive environments. Many studies on the utilization of environmentally ac ceptable inhibitors have reported the successful use of these substances to inhibit corrosion of metals in acidic media [5-6].

MATERIALS AND METHODS

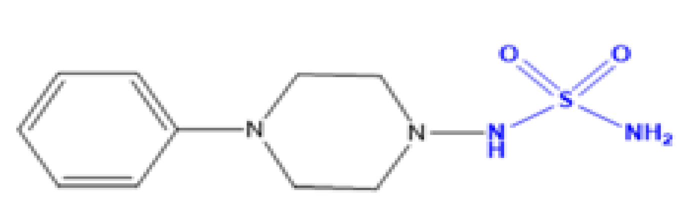

Figure 1. Chemical structure of N-phenylpiperazinylsulfamide

Inhibitor Sample and medium

Corrosion tests were performed on the unalloyed aluminium with 99,98% purity.The aggres sive solution used was prepared by dilution of analytical reagent grade of H2SO4 with distilled water. Inhibitor solutions were prepared in the range, 200 ppm-800ppm concentrations in a 1M H2SO4 solution.

Electrochimicals tests

Polarization measurements were conducted in a conventional three-electrode cell, which includes a working electrode (sample), a platinum counter electrode (CE) and saturated Ag/AgCl reference electrode (RE).Measurements were carried out using SP300 Potentiostat/galvanostat piloted by a microcomputer with EC-Lab V 10.33 Software. The potentials were scanned at a scan rate of 0.5 $\boldsymbol{mV.S^{-1}}$ in the range of -200mV to +200 mV ,The electrochemical impedance spectroscopy, EIS, was carried out with the open circuit potential, Eocp, for each sample; all of the samples were immersed for 60 min over a frequency range of 50 KHz à 10 MHz with a signal amplitude pertu rbation of 10 mV. Next, it was fitted with sets of circuits that give the best value.

RESULTS AND DISCUSSION

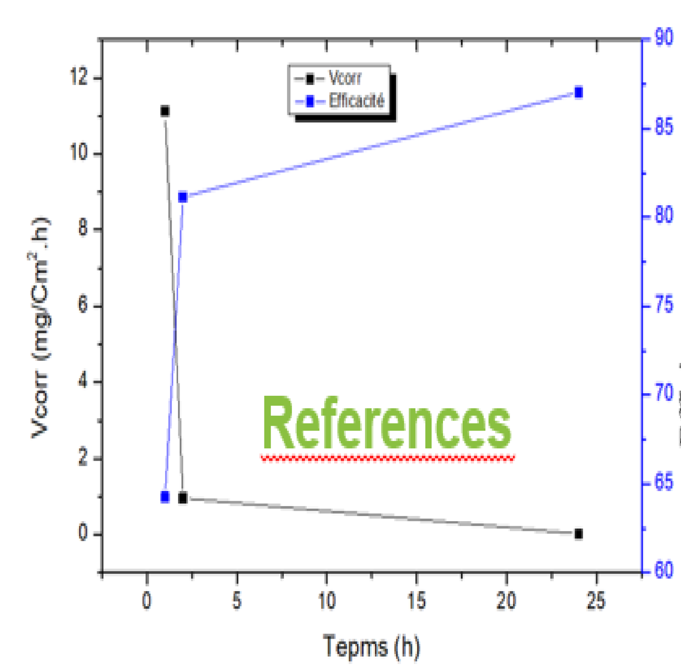

Figure 2. corrosion parameters of aluminium in a 1M H2SO4

The gravimetric data obtained in the absence and presence of N-phenylpiperazinylsulfamide at different Concentrations. The respective corrosion rate illustrated that the addition of Inhibitor molecule decreases hugely corrosion rate. This finding elucidated by Fig.2, confirms that inhibitor adsorbs on aluminium surface and then inhibits the corrosion process. The inhibition efficiency of N-phenylpiperazinylsulfamide with inhibitor concentration to reach higher value (87%) at 800 ppm (Fig. 2). This behaviour indicates that natural molecule acts as an efficient inhibitor for the corrosion of aluminium in H2SO4 media..

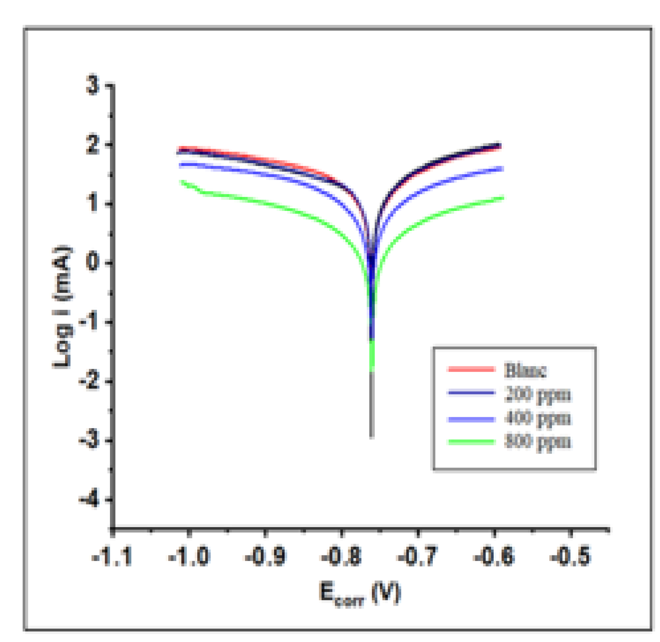

Figure 3. aluminium polarization curves for various in 1M H2SO4 solution

Concentration (ppm)	E_{corr} (mV/Ag/AgCl)	i_{corr} (mA.cm^{-2})	R_p (ohm.cm^2)	β_a (mV)	β_c (mV)	E_{icorr} (%)	E_{Rp} (%)
Blanc	-761.257	4,51007	38,123	48.0	52.2	-	-
200	-760.326	3,75756	45,456	44.1	46.2	16,685	16,132
400	-761.151	2,306386	86,456	58.6	59.8	48,861	55,904
800	-759.853	0,679371	243,123	54.8	58.9	84,936	84,319

Table 1. Electrochemical parametrs and inhibitory effciency of aluminium in 1M HCl without and with the addition on the inhibitor at different concentrations

-*The Icorr values decrease with increasing inhibitor concentration.
-*The Ecorr values were shifted toward the negative in the presence of the inhibitor
The values of βa and βc do not change in a regular way, the inhibitor considered as mixed type inhibitor. According to electrochemical impedance diagrams we found that the charge transfer resistance increases and the capacity of electric double layer decreases when the inhibitor concentration in the solution increases.

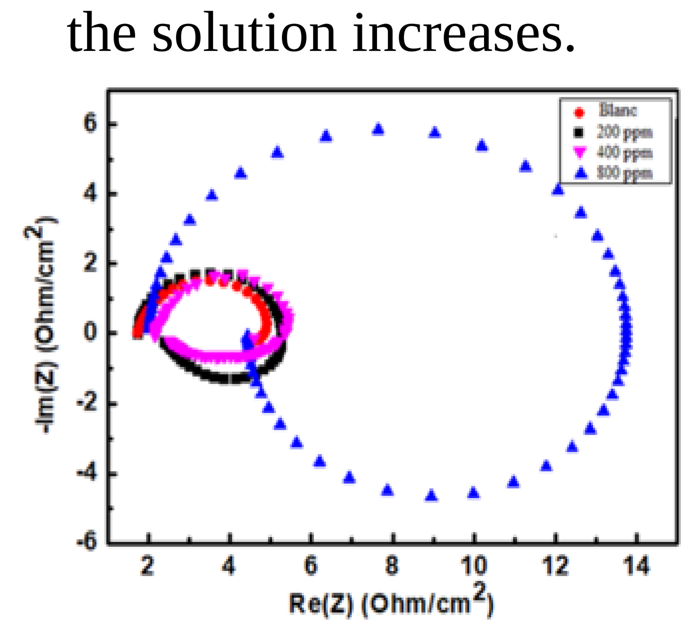

Figure 4. Nyquist impedance diagrams obtained for aluminium at different concentrations of N-phenylpiperazinylsulfamide

The Nyquist curve (Fig. 4) consists of a single capacitive loop with a straight slope at high frequency, indicating that the corrosion reaction is controlled by a charge transfer process and a diffusional process.
Figure 4 inspection reveals that the capacitive loops' diameters grow larger as the concentration of the

CONCLUSION

As conclusion we have demonstrated that:
1 The extract N-phenylpiperazinylsulfamide is effictif inhibiter of corrosion of aluminium in 1M H2SO4.
2. Polarization studies showed that the compounds under investigation were mixed type inhibitors.
3. The weight loss, electrochemical impedance spectroscopy, polarization curves and linear polarization were in good agreement.

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