LOVELY PROFESSIONAL UNIVERSITY

(April-2017)

DISSERTATION-II FINAL REPORT

For the partial fulfillment of the award of degree

Master of Sciences in Chemistry (Honors)

By

Anamika Sethi

Registration No. 11511992

Under the guidance

Of

Dr. Ashish Kumar

School of Chemical and Physical Engineering

TOPIC APPROVAL PERFORMA

School of Chemical Engineering and Physical Sciences

Program : P266-H::M.Sc. (Hons.) Chemistry

COURSE CODE : CHE688 **REGULAR/BACKLOG :** Regular **GROUP NUMBER :** SCRGD0015

Supervisor Name : Dr. Ashish Kumar **UID :** 16464 **Designation :** Associate Professor

Qualification : _____ **Research Experience :** _____

SR.NO.	NAME OF STUDENT	REGISTRATION NO	BATCH	SECTION	CONTACT NUMBER
1	Anamika Sethi	11511992	2015	G1503	9041531741

SPECIALIZATION AREA : Physical Chemistry **Supervisor Signature:** _____

PROPOSED TOPIC : Extraction, isolation and characterization of chemical constituents in common lichen (Usnea) and its anticorrosion and biological activities.

Qualitative Assessment of Proposed Topic by PAC		
Sr.No.	Parameter	Rating (out of 10)
1	Project Novelty: Potential of the project to create new knowledge	7.00
2	Project Feasibility: Project can be timely carried out in-house with low-cost and available resources in the University by the students.	7.00
3	Project Academic Inputs: Project topic is relevant and makes extensive use of academic inputs in UG program and serves as a culminating effort for core study area of the degree program.	7.50
4	Project Supervision: Project supervisor's is technically competent to guide students, resolve any issues, and impart necessary skills.	8.00
5	Social Applicability: Project work intends to solve a practical problem.	7.00
6	Future Scope: Project has potential to become basis of future research work, publication or patent.	7.50

PAC Committee Members		
PAC Member 1 Name: Dr. Gurpinder Singh	UID: 13608	Recommended (Y/N): NA
PAC Member 2 Name: Dr. Ashish Kumar	UID: 16464	Recommended (Y/N): NA
PAC Member 3 Name: Dr. Rekha	UID: 14537	Recommended (Y/N): NA
DRD Nominee Name: Dr. Runjhun Tandon	UID: 19532	Recommended (Y/N): Yes
DAA Nominee Name: Dr. Navneet Singh	UID: 19327	Recommended (Y/N): Yes

Final Topic Approved by PAC: Piracetam as effective corrosion inhibitor for Mild Steel and Aluminium

Overall Remarks: Approved (with minor changes)

PAC CHAIRPERSON Name: 11800::Dr. Ramesh Chand Thakur **Approval Date:** 12 Oct 2016

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Certificate

This is to certify that the pre-dissertation project entitled "**Piracetam as effective corrosion inhibitor for Mild Steel and Aluminium**" submitted by **Anamika Sethi** to the Lovely Professional University, Punjab, India is a documentation of genuine experimental work of coming research work approved under my guidance and is commendable of consideration for the honor of the degree of Master of Science in Chemistry of the University.

_____

Supervisor
Dr. Ashish Kumar
Associate Professor

Declaration

I certify that,

- The work enclosed in this thesis is innovative and has been carried out by me under the guidance of my supervisor, Dr. Ashish Kumar
- The present work has not been submitted earlier to any other university for any degree
- I have been followed the guiding principle provided by the university in the preparation of the report
- Whenever I have used resources (such as data, theoretical representations, any figure, and text) from other sources, I have given due recognition to them by citing them in the report and providing their details in the bibliography.

_____

Date:

Acknowledgement

This project work is the end of my masters' degree in chemistry honors. I have not travelled in a vacuum in this journey. This project report has been kept on track and been seen through to completion with the support and encouragements numerous people including my teachers, my well wishers, my friends. At last of this project work I would like to thank all those people who made this work possible and an unforgettable experience for me.

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I expand my thanks to my friends, family and my roommates who always kept my spirits up with their extended love, affection and support at the time of my project work.

Last but not the least I would like to pay high regards to the authors whose work I have consulted very often during my project work. And I would like to thank Lovely Professional University that provided me the road for the completion of my degree in this particular field.

Anamika Sethi
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M.Sc. Chemistry (hons.)

Contents

PIRACETAM AS AN EFFECTIVE CORROSION INHIBITOR FOR MILD STEEL AND ALUMINIUM

Abstract:

Corrosion being a big issue in today's world it damages the metal and results in the distinct properties of metal. Use of different inhibitors chemical or natural inhibits the corrosion rate to a great extent. The motive of using inhibitors is to increase the life of metals in any way. Corrosion is maintained by the formation of protective layer formed by the category of some compounds that are having heteroatom's in their structures resulting in the protective layer formation which shields the layer of metal from the environment and hence the corrosion is inhibited to some extent. Drugs can be used as an effective corrosion inhibitor. We will conclude the results using various analysis techniques like SEM, EDX, AFM, UV and theoretical studies will be concluded by quantum chemical analysis and Monte Carlo. Piracetam behave as a mixed type of inhibitor and all the kinetic parameters are being calculated in the report.

Introduction

Generally deterioration of metals is known as corrosion by the exposure of external environment on its surface. It is very steady and regular process. Results of corrosion come up with the composition change and may affect the properties of that metal. On exposure with environment or moisture there is slow eating up a metal which reduces its efficiency and effect its physical and chemical properties. This includes a set of reaction which takes place slowly and gradually which results in the formation of rust on the surface of the metal. Malik *et.* al. cited that the corrosion is an electrochemical process which includes a rearrangement of electrons from the metal to the aqueous electrolytic solution[1]. Now a day's corrosion being a very big problem from the house hold to big industries. Chemists are regularly working on it to find new ways and efficient methods to inhibit the growth of corrosion. There are so many methods to prevent

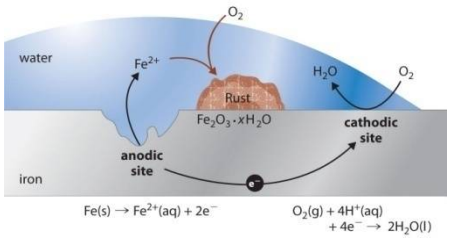
corrosion which include galvanization, cathodic protection etc. but many studies found out that addition of anti-corrosion agents to the place of corrosion have a effective application against its protection[1]. Addition of inhibitors to the metal can prevent or stop the corrosion activity on the metal surface.[1] An effective inhibitor is one which is used in low concentrations. Corrosion results in a great loss in economy as it deteriorate the metals present in aircraft, ships, plumbing etc. So here we need an immediate and effective method to prevent corrosion. Anti corrosion substances can be synthesized by using many materials. Malik *et.* al used surfactants as a anti-corrosion material[1]. He studied that the surfactants shows a better anti corrosion activity. Surfactants formed micelles and get adsorbed on the surface of the metal which prevents the interaction of the metal with the outer environment.[1] Adsorption of the surfactant on the metal surface is given by the equation[1]:-

$$\text{Surfactant(sol.)} + \text{nH2O(ads.)} \rightarrow \text{Surfactant(ads.)} + \text{nH2O(sol.)}$$

Cristofari *et.* al. studied the anticorrosion activity on mild steel they concluded that the anti-corrosion activity is shown by organic compounds[2] having heteroatom's as their main composition[2]. Finsgar *et.* al. studied the corrosion inhibitors of lower grade steel in acidic media[3].

Types of corrosion:-

- **General corrosion**: It is an electrochemical phenomenon in which the reactions start over entire surface of the metal at almost same rate. General corrosion results in leakage through the metal surface because it reduces the mechanical thickness of metal.



http://www.hkdivedi.com/2015/11/different-forms-of-corrosion.html

Figure 1: General Corrosion

- **Pitting corrosion**: Occurs on the small spots of metal surface at a high rate. The flaws present in the coating of metal surface are usually the place where pitting corrosion occurs. It is also common in corrosion resistant metals that form native oxides on their surface.

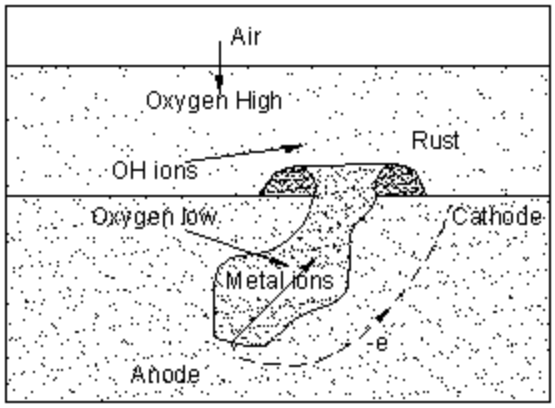


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Figure 2: Pitting Corrosion

- **Crevice corrosion**: In certain metals the surface is not uniform and consists of certain occluded regions called cervices. As this metal comes in contact with the environment, the environment of this region does not freely mix with the bulk environment and this difference leads to corrosive attack.

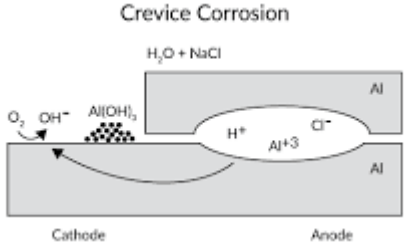

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Figure 3: Crevice Corrosion

- **Inter granular corrosion**: In some engineering alloys the surface of the metal is solidified by coating it with some melt consisting of mixture of elements. As a result of which there comes a difference between properties and the chemical composition of these solid crystals and the inside of metal surface. This result in the rapid corrosion between these crystals called intergranular corrosion.

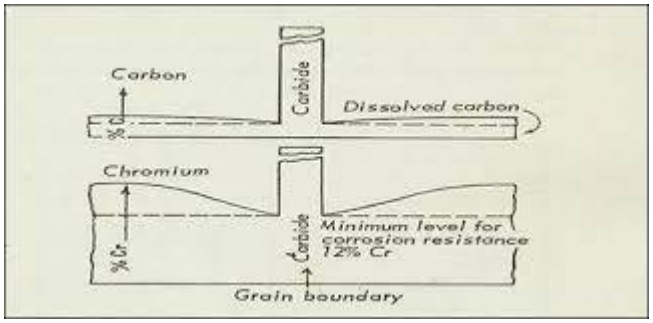

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Figure 4: Intergranular Corrosion

- **Environmentally induced corrosion**: When some metals are exposed to chemically reactive atmosphere, formation of crack occurs due to the application of mechanical stress. Organic solvents, aqueous solutions have been known to be a main cause of this failure.

http://www.hkdivedi.com/2015/11/different-forms-of-corrosion.html

Figure 5: Environmentally Induced Current

- **Dealloying**: Some alloys are made up of different elements and when dealloying is done it includes the leaching of one of the alloys which reduces the mechanical strength and leads to porous surface.

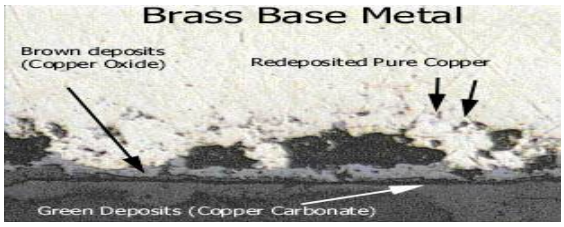

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Figure 6: Dealloying

- **Galvanic corrosion**: Different alloys have different chemical and electrochemical properties so joining of these dissimilar metals leads to the completion of electric circuit through the joint and the environment increase the corrosion rate of highly reactive metals.

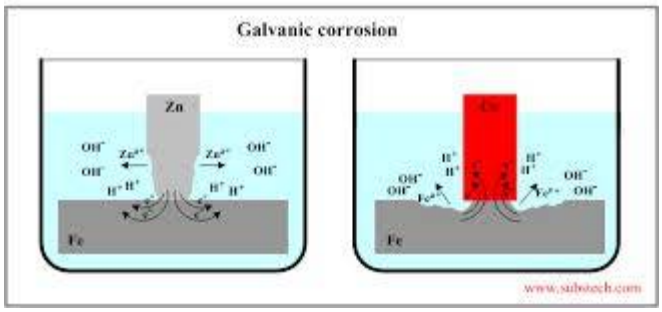

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Figure 7: Galvanic Corrosion

- **Erosion corrosion**: According to Derrick H. Lister, Erosion corrosion occurs as a result of high relative motion between the metal and the environment. Erosion corrosion leads to the formation of holes, cavities and grooves on the metal surface aligned in the direction of fluid.

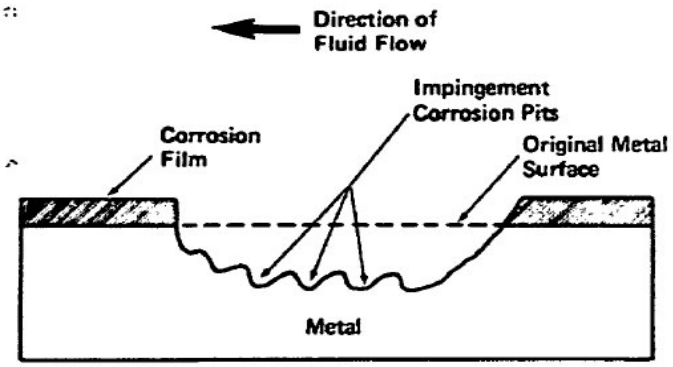

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Figure 8: Erosion Corrosion

Review of literature

Various studies have been done by using the pharmaceutical compounds as corrosion inhibitors. Owing to their structural similarities to the commercially used corrosion inhibitors and non-toxic behavior these have proved to be a great breakthrough in the formation of environmentally safe corrosion inhibitors. The techniques usually used involve weight loss, polarization techniques and electron impedance spectroscopy. The efficiency of inhibition and the surface coverage are estimated from weight loss method by using the formula:

$\Theta = W_0\text{-}W_i/W_0$

$\eta_w\% = W_0\text{-}W_i/W_0$

Where W_0 and W_i are the weight loss in absence and presence of inhibitor, $\eta_w\%$ is the inhibition efficiency and Θ is the surface coverage. Studies have been done using drugs as environmental friendly corrosion inhibitors.

Abdulrasoul Salih Mahdi [4] reported amoxyllin, an antibacterial drug as a corrosion inhibitor of steel in alkaline media. The techniques used involved potentiodyanamic polarization. Result suggested concentration of inhibitor is directly proportional inhibition efficiency and inversely proportional to current density. Amoxicillin was found to be a mixed type inhibitor through travel curves. The corrosion efficiency was found out to be 95.03% at a concentration of 2.5g/l of amoxicillin. I.A. Adejoro[5] *et.* al. reported the anticorrosion activity of ampllicin, an antibiotic drug on the corrosion of mildsteel in acidic media by using gravimetric method. It was found that with increase in the concentration of inhibitor is directly proportional to the inhibition efficiency and temperature is inversely proportional to the inhibition efficiency. Ampllicin showed the inhibition efficiency of 75.85% at 30oc.the HOMO and LUMO plots further suggested that ampllicin is an effective inhibitor. Rupesh Kushwa[6] *et.* al. used aspirin as an ecofrienly corrosion inhibitor of mild steel using acidic medium. Results showed that concentration of

inhibitor is directly proportional to the inhibition efficiency. Aspirin was shown to adsorb on the surface of metal by Langmuir adsorption isotherm. Temperature and activation parameters were also estimated. L.Magaji, P.O Ameh, N.O Eddy, A.Uzairo, A.Saika, S.Habib, A.M Ayouba, and S.M Gumel[7] reported the corrosion inhibition of ciprofloxacin as a corrosion inhibitor of mildsteel in acidic medium. The techniques used involved weight loss, thermometric and scanning electron microscopy techniques. It was shown that inhibition efficiency is directly proportional to the inhibitor concentration and inversely proportional to the temperature. The adsorption of ciprofloxacin on mildsteel was found to obey Langmuir adsorption isotherm. S.Harikumar and S.Kartheykaren[8] used antibiotic drug cloxacilin as corrosion inhibitor of mildsteel in acidic medium. The techniques included weight loss, electron impedance spectroscopy, and tafel polarization and hydrogen permeation studies. At the concentration of 15×10^{-4} M of inhibitor , the inhibition efficiency was found out to be 81%.the adsorption of this compound on mildsteel was found to follow tempkin adsorption isotherm. Ambrish Singh, Ashish Kumar Singh and M.A Quraishi[9] studied Dapsone drug as a corrosion inhibitor of mild steel in acidic medium. The techniques used were weight loss, electrochemical impedance spectroscopy, tafel polarization and polarization resistance. Results showed that Dapsone acts as a mixed type inhibitor, particularly cathodic with HCl and anodic with H2SO4.the adsorption of Dapsone on surface of mildsteel followed Langmuir adsorption isotherm. Factors like enthalpy, entropy, activation energy and Gibbs free energy was also calculated in order to know the mechanism of reaction. R.S Abdul Hameed, H.I Alshfey, A.H Abunawas[10] reported expired diclophen as corrosion inhibitor of mildsteel in HCl. The drug was found out to be mixed type inhibitor by using potentiodynamic measurements. More is the inhibitor concentration, more is inhibition efficiency. It was found that the inhibitor adsorbs mildsteel surface by following Langmuir adsorption isotherm. Thermodynamic parameters were also calculated. P.Geethamani, P.K Kasturi, S.Aejitha[11] reported the anticorrosion effect of expired drug of asthaline expectorant on mildsteel. The techniques used involved weight loss and electrochemical methods. Results suggested that, as concentration of inhibitor, immersion time and temperature were increases the inhibition efficiency also increased. Asthaline acted as mixed type inhibitor by polarization techniques. Results showed that asthaline followed Langmuir, freundlich and tempkin adsorption isotherm. Husin I.Al-Shafey, R.S Abdel Hameed, F.A.Ali, Abd el-Aleem, S.Abdoul-Magd and M.Salah[12] Studied the anticorrosion effect of expired phenytoin sodium drug on carbon steel in

acidic medium. The techniques used involved using weight loss, electrochemical spectroscopy, polarization techniques and scanning electron microscopy. PSD followed Langmuir adsorption isotherm. Polarization curves suggested PSD to be a mixed type inhibitor. N.O Eddy, S.A Odoemelam and P.Ekwumemgbo[13] studied the inhibitive behavior of Penicillin G on surface of carbon steel in acidic medium. The inhibition efficiency of penicillin G was found to be directly proportional to the concentration of inhibitor and inversely proportional to the temperature. Results showed that adsorption of Penicillin G followed Langmuir adsorption. Imran Reza, Ejaz Ahmad and Farhan Kareem[14] reported piperacillin sodium as a corrosion inhibitor of mildsteel in acidic medium. The studies involved weight loss and electrochemical techniques. It was concluded that the efficiency of inhibition to be 93% at 7.2×10^{-4} M concentration of piperacillin.polarizataion techniques confirmed that the inhibitor is a mixed type. And the adsorption of piperacillin on the surface of mildsteel obeys Langmuir adsorption isotherm. S.Mani megalai, R.Ramesh and P.Manjula[15] studied the anti corrosion activity of trazodone ton mildsteel in acidic medium. The techniques involved weight loss method. It was seen that the inhibition efficiency increases was directly proportional to the concentration of inhibitor.. The adsorption of trazodone on the surface of mildsteel was shown to follow Langmuir adsorption isotherm. Trazodone was shown to have an inhibition efficiency of 98% at the concentration of 8.8×10^{-4} M. A. Samide, B. Tutunaru, and C. Negrilab[16] studied the anticorrosion activity of sulfa drug on steel in acidic medium. The sulfa drug called sulphathiazole was used and the techniques involved weight loss and electrochemical methods.XPS was used to analyze the surface chemistry. TBSA inhibits corrosion of carbon steel in 1.0 mol L^{-1} HCl solution; it has an efficiency of 86.7 ± 1 % obtained from mass loss data and electrochemical measurements. N. O. Eddy, S. A. Odoemelam and A. J. Mbaba[17] reported sporfloxacin as corrosion inhibitor of mildsteel in acidic medium. Techniques used were gasometric, gravimetric and thermometric methods. Inhibition efficiency was reported to vary from 79.68% to 82.30%. With increase in concentration of sporfloxacin, the inhibition efficiency increased while as with increase in temperature, it decreased. The adsorption of sporfloxacin on the surface of mildsteel was found to follow Langmuir adsorption isotherm. M. Abdallah[18] studied the corrosion inhibition by using anti-bacterial drugs for aluminium in hydrochloric solutions. He used many methods including hydrogen evolution[18], weight-loss[18] and potentiostatic[18] techniques and found out that the inhibitor efficiency depends upon the concentration and the structure of the anti-bacterial drugs.

He also cited that the inhibitive properties of the drugs are because of blocking of electrode site by the adsorption of the molecules on the metal surface. The results of following experiments are such that the inhibition efficiency of the drugs increased by increasing the electron donor[18] characteristics of the groups attached to the structure of the drug and on decreasing the temperature[18]. The adsorption of the following drug obeys the Langmuir adsorption isotherm[18]. M.A. Quraishi *et.* al. studied the action of barbiturates[19] as an effective corrosion inhibitor for mild steel in acidic media. They synthesized the set of barbiturates and studied their corrosion inhibition efficiency using electron impedance spectroscopy[19], tafel polarization technique[19], weight-loss[19] studies and observed that the adsorption follows the Langmuir[19] adsorption isotherm. He concluded in his studies that the all four arylidiene barbiturates[19] shows good corrosion inhibition efficiency in the range of 89-97%. The result of inhibitors are such that they behave as both anodic and cathodic inhibitors so called as mixed type[19] of inhibitors. The results drawn from the experimental data is in good agreement with each other. L.Majidi[20] *et.* al. studied that the carveol derivatives can also behave as anti-corrosion material on steel in 1M hydrochloric acid[20] he reported maximum corrosion inhibition up to 79.6% by using weight loss measurements at 313-323K. The adsorption obeys Langmuir isotherm and the respective kinetics measurements are done[20]. He concluded that the inhibition efficiency increased by increasing temperature and by increasing the concentration of inhibitors. Ashish Kumar Singh[21] *et.* al. studied the inhibition effect of cefazolin[21] of mild steel in hydrochloric solution (1M). Many other techniques like electron impedance, potentiostatic, atomic force microscopy[21] has been done by these co scientists. They withdrew the results that the corrosion inhibition increases with the increase in the concentration of the inhibitor. They also verified that the adsorption of cefazolin on mild steel does obey the Langmuir adsorption isotherm and they also calculated the thermodynamic parameters and concluded that the cefazolin act as a mixed type of inhibitor predominately controls cathodic reaction[21]. They also concluded that with the increase in temperature the corrosion inhibition efficiency decreases which further lead to increase the activation energy of the corrosion process. The adsorption process involved in the reaction is spontaneous and exothermic in nature and also there is increase in the entropy of the reaction which further supports the spontaneity of the corrosion process[21]. Imran *et.* al. studied the corrosion inhibition on mild steel in acidic media using cefixime[22] as an corrosion inhibitor. They investigated that at 303K the inhibitor shows >90% inhibition efficiency and the inhibitor

works by adsorption on the surface of mild steel and follows Langmuir adsorption isotherm. The efficiency of the inhibitor decreased as there is increase in temperature and cefixime act as a mixed type of inhibitor. Priyanka Singh[23] *et.* al. investigated the corrosion inhibition of cetirizine[23] on mild steel in acidic media. They investigated that cetirizine behave as very good corrosion inhibitor even at very low concentration of 100ppm. They also studied the quantum chemical, weight-loss and electrochemical measurements for this type of inhibitor and concluded that cetirizine behave as mixed type of inhibitor and the quantum chemical studies are applied to find out the adsorption pattern of cetirizine on the surface of mild steel[23]. Cetrizine on increasing concentration behave as a good corrosion inhibitor and shows up to 95% efficiency at 100ppm. The results drawn from the thermodynamic parameters shows that negative value of ΔG which tells about the spontaneity of the adsorption[23]. Ambrish Singh[24] *et.* al. studied the corrosion inhibition of cemtidine[24] for mild steel in 1M acid concentration. Cemtidine behave as a mixed inhibitor[24]. Gece Gokhan studied the corrosion efficiency of drugs and saw that the atoms generally have π-bonds in their structure behave as a good corrosion inhibitors[25] and the donation of electrons form the pi-system is responsible for showing the anti-corrosion behavior. Obot *et.* al. studied the aluminium corrosion in 0.5M HCl solution. Fluconazole[26] is being studied as an anti-corrosion material and found that the inhibition efficiency increases with the increase in concentration of drug and decreases with the decrease in temperature. M.Abdallah, I Zaafarany, S.O.Al-Karanee, A.A. Abd El-Fattah[27] reported the corrosion inhibition of Al and Al alloys with some hypersensitive drugs as corrosion inhibitors in aqueous medium. It was found that rate of corrosion increased with increase in the concentration of acid. Results showed that the inhibition efficiency was directly proportional concentration of inhibitor. The adsorption process was found to follow Langmuir adsorption isotherm. Hadeel Adil[28] reported gaufenisin drug as a corrosion inhibitor of zinc in acidic medium. Techniques included weight loss method. The results showed that with increase in the concentration of inhibitor, the inhibition efficiency increases. The inhibition efficiency was found out to be 81% at 300 ppm concentration of inhibitor. R.S .Abdel Hameed, E.A.Ismail, A.H.Abu-Nawwas and Husin I.Al-Shafey[29] reported expired voltarin drug as corrosion inhibitor of Aluminuim in acidic medium .the electrochemical and weight loss methods were used and results from polarization curves indicated that the expired drug voltarin acts as a mixed type inhibitor. Results showed that Langmuir adsorption isotherm was being followed. Thermodynamic parameters revealed that adsorption is spontaneous and exothermic. It

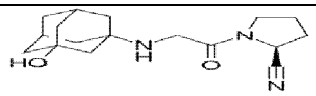
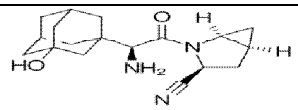
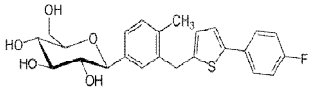
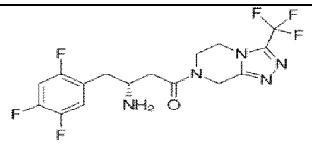
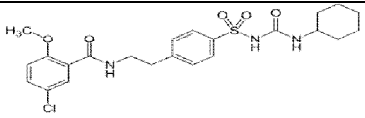
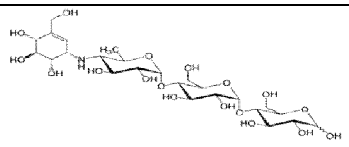
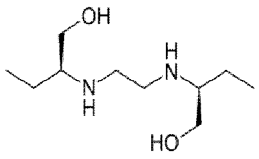
was seen that inhibition efficiency increased with increase in inhibitor concentration and decrease in temperature. Mudigere Krishnegowda Pavithra, Thimmappa Venkatarangaiah Venkatesha, Mudigere Krishnegowda Punith Kumar and Nanjanagudu Subba Rao Anantha[30] reported the use of doxycycline hydrochloride drug as corrosion inhibitor of Almunuim .potentiodynamic polarization, chronoamperometry; EIS were used for the studies. It was seen that inhibition efficiency was 90% in 3.5% NaCl. Results suggested that adsorption followed Langmuir adsorption isotherm. The mode of adsorption was seen to be both physisorption and chemisorption.

Based upon the above literature, much work has been done using pharmaceutical compounds as corrosion inhibitors. But very less work has been done on corrosion inhibition using Antidiabetic drugs. In order to carry forward our project; we have made a choice of some common drugs which can be used as corrosion inhibitors. The effect of corrosion inhibition by the drugs shall also be compared to the effect of antioxidants on the corrosion inhibition of steel and aluminium. The parameters I have taken into consideration include:

- The drugs that we have selected are easily available.
- They are non-toxic and have almost negligible effect on environment
- They are water soluble
- They have a structural similarity to the corrosion inhibitors used. They contain heteroatoms like N,S and O in their structure.
- They are cheap.
- And finally no work has been reported on these drugs till now.

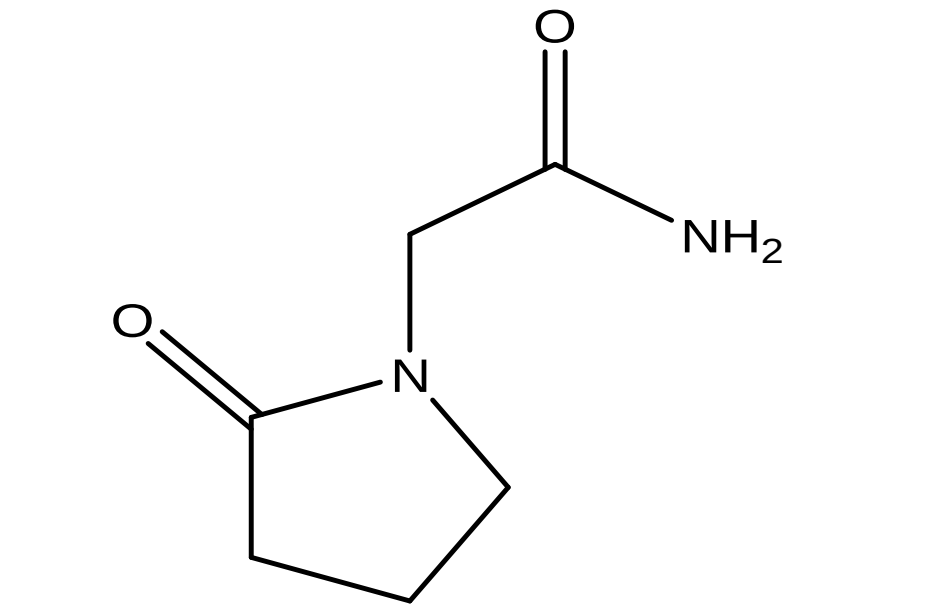
The shortlisted drugs to be worked on are: vildagliptin, saxagliptin, Canagliflozin, Sitagliptin, glyburide, Acarbose, Ethambutol. The anti oxidant to be used includes 2,2-diphenyl-1-picrylhydrazyl(DPPH).The table below shows the drugs, their structures, properties and solubility.

Table 1: Review Of some Drugs

Name	Structure	Heteroatoms	Solubility	Property
Vildagliptin		N,O	Water soluble	Antidiabetic
Saxagliptin		N,O	Water soluble	Antidiabetic
Canagliflozin		S,O	Water soluble	Antidiabetic
Sitagliptin		N,O	Water soluble	Antidiabetic
Glyburide		N,O,S	Water soluble	Antidiabetic
Acarbose		N,0	Water soluble	Antidiabetic
Ethambutol		N,O	Water soluble	Antimycobacterial

RESEARCH BACKGROUND:

- Taking into considerations the above mentioned effects of corrosion it is important to take a pledge to inhibit this process. Although it cannot be eliminated completely but we can make an attempt to atleast inhibit its rate at which it takes place. Various corrosion inhibitors are present some of which can be discussed. A corrosion inhibitor can be termed as a substance which decreases the corrosion rate upon its addition to the environment.
- Anodic corrosion inhibitors reduce the corrosion by forming an oxide layer on the metal as a result of retarding anodic reactions. It leads to the anodic shift which forces the equilibrium to shift to passivation zone thus decreasing the corrosion rate. Commonly used anodic inhibitors are chromates, tungstates, molybates and phosphates.
- Many scientists however have cited much articles in the field of corrosion inhibitors as plant extracts, drugs and many more work as to see the efficiency of corrosion inhibitors in different media. A material to behave as a good corrosion inhibitor should have a heteroatom in as their constituent in structure. It has been studied that the donation of pair of electron from the heteroatom itself results into formation of a layer onto the surface of metal and the metal is being protective by the outside moisture and as a result the corrosion is retarded on metal surface. Annually many drugs get their expiry date and hence are wasted as they are not beneficial for human intake. But if we use these drugs in different manner the drugs can be utilized as corrosion inhibitors. So far many drugs have been studied and yielded a very good efficiency such as amoxicillin, cefazolin, cemitidine, cetirizine, sporfloxacin etc. Piracetam being chosen for this experiment as it contain N, O as an active ingredient in their structure which fulfil the criteria for being a good corrosion inhibitor having molecular formula $C_6H_{10}N_2O_2$. Molecular weight: 142.16g/mol. Bioavailability is 100% and is olt under the brand name Biotropil.



2-(2-oxopyrrolidin-1-yl)acetamide

Figure 9: Structure of Piracetam

RESEARCH METHODOLOGY:

We can study the corrosion inhibition efficiency by number of ways including:

- ✓ Weight loss studies
- ✓ Electrochemical measurements(EIS)
- ✓ Quantum chemical analysis
- ✓ Polarization methods
- ✓ Montecarlo simulation
- ✓ UV
- ✓ IR
- ✓ SEM/EDS
- ✓ AFM

- **Weight loss method: -** Cristofari *et.* al. cited his work in the corrosion measurement of steel in 0.5M H_2SO_4 solution using weight loss method at 298K after 6hours of immersion period[2]. The equation for the weight loss measurements is given by:-

$$W = \Delta m / St \text{ --------- } (1)^2$$

$$Ew\% = \frac{Wcorr - Wcorr.inh}{Wcorr} \times 100 \text{ ---------- } (2)^2$$

- **Electrochemical Impedance Studies: -** EIS300 software is as Gamrys impedance spectroscopy package. Impedance measurements shall be calculated from this instrument.

Charge transfer resistance values are calculated from the high frequency impedance values. Inhibition efficiency is calculated from the values of corrosion current density.

Inhibition efficiency is calculated from the values of corrosion current density. This can be shown by the following equation:

$$\eta_p\% = \frac{iocorr - icorr}{iocorr \times 100}$$

Where $\Pi_p(\%)$ is the inhibition efficiency and i_0 corr and icorr are the corrosion current density without and with inhibitor respectively.

- **Polarization techniques:** This technique is used in order to know the values of corrosion potential (Ecorr), current densities (I corr), anodic tafel slopes (βa), cathodic tafel slopes (βc), surface coverage (θ) and inhibition efficiency as a functions of inhibitor concentration

- **Quantum Chemical Analysis:-** Elmsellem *et.* al. studied the anti-corrosion activity on steel and studied quantum chemical analysis method applying density functional theory[31]. His study include quantum parameters like highest occupied molecular orbital (HOMO)[31], lowest unoccupied molecular orbital(LUMO)[31], dipole moment[31] and amount of electrons transferred[31]. In order to find the HOMO, LUMO and dipole moment of the inhibitors Gaussian software shall be used. This program runs. By using density function theory method.

- **SEM and AFM: -** After experiment we are going to study or compare the erosion of the surface of metal using these techniques. These techniques give the information about the surface morphology of the metal. AFM gives the detailed image of metal being eroded and in comparison with that of metal in the inhibitor media.

EXPERIMENTAL DETAILS:

1. **Materials required**: - Metal sheets of both aluminium and mild steel is bought from the local shops and are made to cut into 2*2cm dimension and are supposed to abraded to remove the upper coating from them with the help of emery paper of grade number 100 and 220.
2. **Solutions**:- The acid solutions are made (1M, 2M, 3M, 4M, 5M, 6M, 7M) using Rankem Chemicals
3. **Weight Loss method**: - Firstly, the acid is standardized from 1M-7M H_2SO_4 and simultaneously for HCl. Taking 7M as a standard acid the further weight loss studies are carried out. From acid standardization we got 62% weight loss and then inhibitor variation is done from 200ppm to 4000ppm concentrations. We got good results in 4000ppm concentration for 3h at 303K.

$$W = \Delta m/St \text{ --------- } (1)^2$$

$$Ew\% = \frac{Wcorr - Wcorr.inh}{Wcorr} \times 100 \text{ ---------- } (2)^2$$

4. **UV Analysis:-** The UV Analysis is donr from the department of chemical and physical sciences, Lovely Professional University, using SHIMADZU UV-1800 spectrophotometer.

5. **Quantum chemical Studies:-** Quantum chemical analysis was performed using the MNDO and AM1 method of the quantum chemical package MOPAC 6.0 of Hyperchem 7.5. The algorithm used for computation was Polak- Rieberre, which is fast and accurate. Geometry optimization was performed on Piracetam inhibitor using DFT employing the BLYP functional together with the generalized gradient approximation (GGA) using the DNP basis sets. A vibrational analysis was carried out for each optimized molecules to ensure that they are at a minimum on the potential energy surface (no imaginary

frequency). The convergence criteria and the global orbital cutoffs were set to "fine" before the calculations. The tolerances of energy, gradient, and displacement convergence were 1 × 10 -5 Ha, 2 × 10 -5HaÅ-1and 5 × 10 -3 Å, respectively. Direct inversion in an iterative subspace (DIIS) and an orbital occupancy smearing parameter of 0.005 Ha were used to speed up SCF convergence. The effect of aqueous solvent was simulated by re-optimizing all the geometries at the BLYP/DNP level using the COSMO (conductor-like screening model).

6. **Monte Carlo Analysis** :- Monte Carlo simulations using the Adsorption Locator and Forcite codes implemented in the Material Studio 6.0 software from Accelrys Inc. USA was adopted to compute the adsorption energy of the interaction between Piracetam and Fe surfaces. For the whole simulation procedure, the Compass force field was used to optimize the structures of all components of the system of interest. The simulations were carried out in the simulation boxes (42Å× 42Å × 55Å) having α= 90.00o; β = 90.00o and γ = 90.00owith periodic boundary conditions in order to simulate a representative part of an interface devoid of any arbitrary boundary effects. The Al (111) planes were next enlarged to a (10× 10) super cell. After that, a vacuum slab of 50Å thickness was built above the surfaces to convert the system to 3D periodicity. The optimized inhibitor using the Forcite code was then added near the surface of Fe(110)and a Monte Carlo simulation annealing procedure was carried out.

RESULTS AND DISCUSSIONS FOR STEEL

WEIGHT LOSS STUDIES: The most convenient and easy method for studying corrosion inhibitor efficiency. Weight loss of different samples of steel and aluminium are being studied in the presence and absence of inhibitor.

The weight loss results of acid variation are given below:

Table: 2 Acid Variations

Concentration	Initial weight	Final weight	Weight loss	%weight loss
1M	1.3687	1.3278	0.0409	2.9882
2M	1.332	1.2764	0.0556	4.1741
3M	1.238	1.097	0.141	11.3893
4M	1.38	1.138	0.242	17.5362
5M	1.4147	0.9937	0.421	29.7589
6M	1.3709	0.7971	0.5738	41.8557
7M	1.2951	0.4982	0.7969	61.5319

From the above table it has been drawn that the as we increase the concentration of acid from 1M to 7M the effect on weight loss is continuously seen and there is increase in percentage weight loss and the maximum weight loss is seen in 7M concentration viz. 61.53%

Piracetam:

The weight loss studies are further carried out for 200, 400, 800, 1000, 2000, 3000, 4000ppm concentration of inhibitor and the results came out to be shown in the following table.

Table 3: Inhibitor variation

Concenration	Initial Weight	Final weight	Weight Loss	% wt loss	Inhibition Efficiency
200	1.4474	1.0564	0.391	27.0139	53.4080
400	1.4241	1.1244	0.2997	21.0448	64.2874
800	1.47	1.2602	0.2098	14.2721	75.0000
1000	1.4808	1.3102	0.1706	11.5207	79.6711
2000	1.2867	1.1286	0.1581	12.2872	81.1606
3000	1.3822	1.2864	0.0958	6.9309	88.5843
4000	1.4403	1.3805	0.0598	4.1519	92.8741
Blank(7M)	1.3463	0.5071	0.8392	62.3338	

The results drawn from the above table is that the inhibitor at 4000ppm gives the most efficient results as the value of inhibition efficiency(η%) is 92.8741%. the reason may be the increase of adsorption onto the surface of steel. The overall discussion from this table is that when the

concentration of inhibitor is increased from 200 to 4000ppm the percentage efficiency is increased.

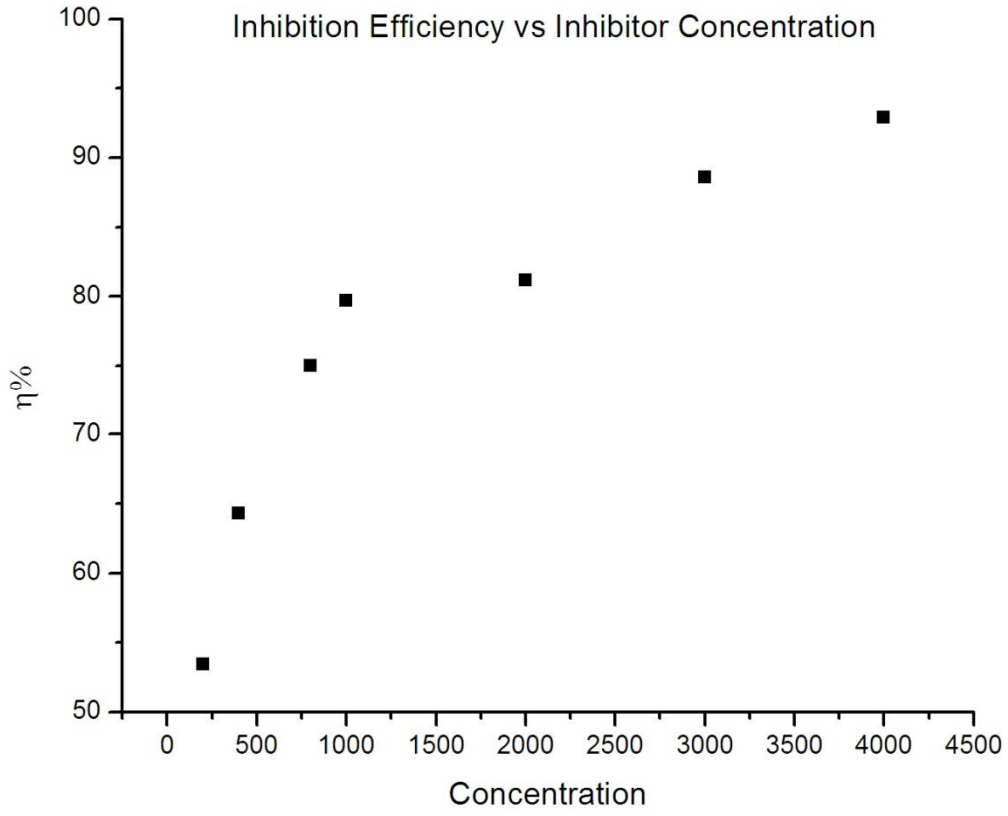


Figure10: Inhibitor efficiency vs Inhibitor concentration

Effect of temperature:

The effect of temperature is seen by continuing the same weight loss experiments in different temperatures viz. 293K, 298K, 303K, 308K, 313K and it has been observed that the firstly the efficiency is increased to a certain temperature i.e. 303K but after that temperature the inhibition efficiency decreased. The results are shown in following table.

Table 4: Temperature Variation

Temperature		Initial weight	Final weight	Wt. loss	%wt loss	Inhibition efficiency
20	Blank	1.5854	1.3932	0.1922	12.1231	33.9229
	Inhibitor	1.5197	1.3927	0.1270	8.3569	
25	Blank	1.4119	0.8727	0.5392	38.1896	60.0704
	Inhibitor	1.5342	1.3189	0.2153	14.0333	
30	Blank	1.4437	0.5372	0.9065	62.7900	92.0463
	Inhibitor	1.4923	1.4202	0.0721	4.8314	
35	Blank	1.4586	0.3694	1.0892	74.6743	78.9019
	Inhibitor	1.4730	1.2432	0.2298	15.6008	
40	Blank	1.5585	0.1627	1.3958	89.5604	37.4337
	Inhibitor	1.2480	0.3747	0.8733	69.9759	

Further, corrosion rates are being calculated by using by formula :

$$C_R = \frac{wt\ loss(g) \times k}{alloy\ density(\frac{g}{cm^3}) \times A \times time(hr)}$$

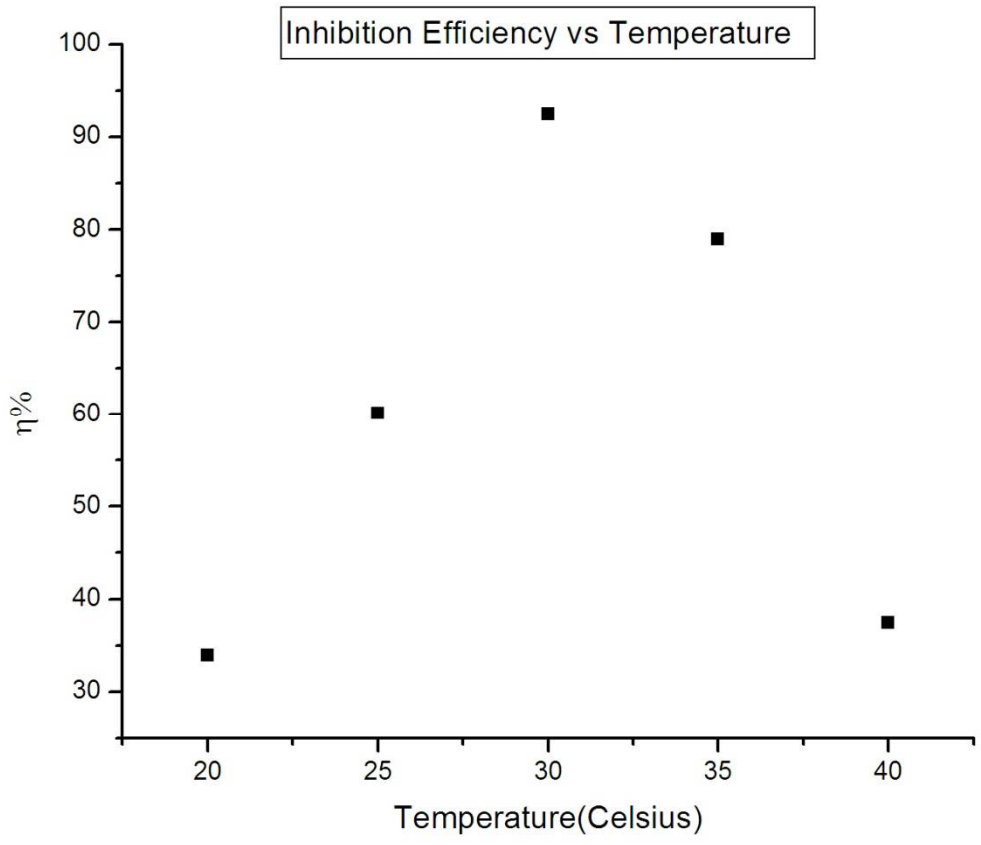


Figure 11: Inhibition Efficiency vs Temperature

The time dependent studies are also being done on mild steel using the inhibitor Piracetam and the results are such that the inhibitor efficiency increases when we increase the time of emersion. The following table gives the description of statement written above.

Table 5: Time Variation

Time(hr)		Initial weight	Final weight	Wt. loss	%wt loss	Inhibition efficiency
1	blank	1.3392	1.2264	0.1128	8.4229	
	inhibitor	1.2303	1.1993	0.0310	2.5197	72.5177
2	blank	1.4003	1.0974	0.3029	21.6310	
	inhibitor	1.3058	1.234	0.0718	5.4985	76.2958
3	blank	1.4381	0.5383	0.8998	62.5686	
	inhibitor	1.5321	1.4635	0.0686	)4.4775	92.3760
4	blank	1.4814	0.2394	1.2420	83.8396	
	inhibitor	1.4133	1.3672	0.0461	3.2618	96.2882

Adsorption isotherms can also be used to explain the nature of interaction between the inhibitor molecules and the metal surface as during the process of weight loss studies the inhibitor is adsorbed on the surface of the metal. The values of surface coverage (θ), corresponding to that of different inhibitor concentrations at 303K was taken to get the isotherm.
The adsorption isotherms generally used are: -

Langmuir isotherm, $\frac{\theta}{1-\theta} = K_{ads}C$

Freundlich isotherm, $\theta = K_{ads}C$

where, $K_{ads.}$ Is the equilibrium constant, C is the inhibitor concentration and θ is the surface coverage.

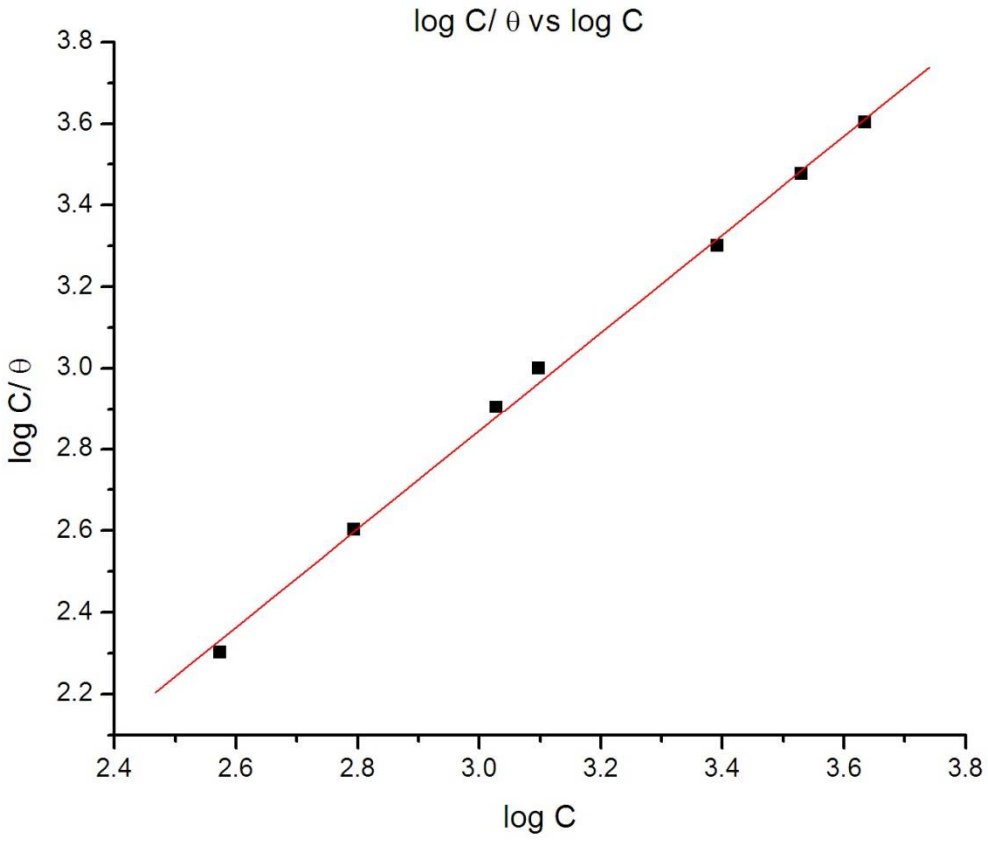


Figure12: Langmuir Isotherm

The slope of above variation is almost equal to 1, which indicates that the Langmuir adsorption isotherm is obeyed for the adsorption of Piracetam on the surface of the metal. The graph itself shows the linearity in the trend.

Arrhenius equation is used to calculate the activation energy of the process: -

$$C_R = A \exp(-Ea/RT)$$

The symbols have their usual meanings.

A - Arrhenius Equation

E_a – Activation Energy

C_R- Corrosion Rate

R- Rate Constant

T- Temperature

Sample	E_a(kJ/mol)	ΔH(kJ/mol)	ΔS($kJmol^{-1}K^{-1}$)
Blank	55.92	24.8041	11.71660675
Piracetam	127.27	55.51	44.68

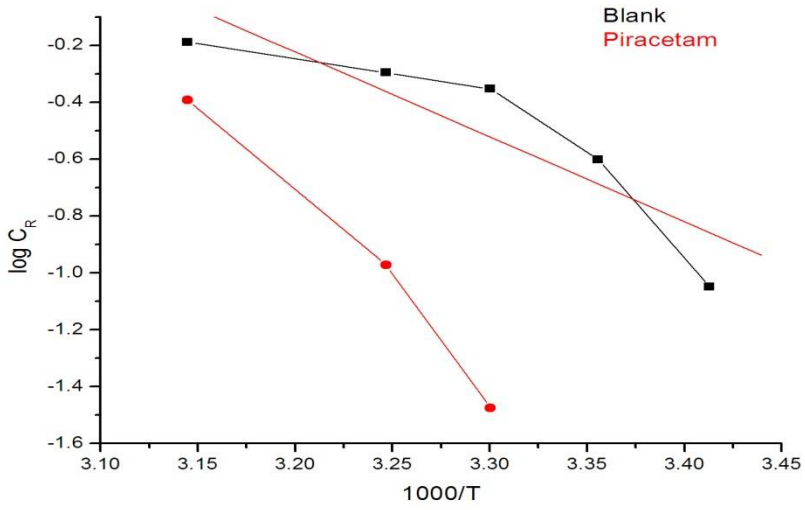


Figure13: Activation energy blank vs. inhibitor

Thermodynamics studies: - The data obtained from thermodynamics parameters plays a very important role in deciding the role of inhibitor effective for corrosion studies. Various parameters like gibb's free energy, entropy, enthalpy and heat of adsorption. The formula used for calculating the gibbs free energy is as follows: -

$$\Delta G^0_{ads} = -2.303RTlog(55.5Kads)$$

where, T is the temperature of the system and the constant value 55.5 is the molar concentration of water. To get spontaneos reaction the value of ΔG should come out to be negative. The ΔG is coming out to be -13.086 $kJmol^{-1}$ for inhibitor which explains the electrostatic interaction

between the charged metal surface and the charged organic molecules present in the drug. From the equation: -

$$lnkads = -(\Delta H^0_{ads}/RT) + C$$

It is clear that (ΔH_{ads}/R) gives the slope of the equation when the graph is plotted between ln K_{ads} vs. 1000/T. the graph comes out to be straight line and the slope gives the respective values. In the equation, R is the universal gas constant, T is temperature of the system, ΔH_{ads} is the heat of enthalpy of the system.

Table 6: Thermodynamic Parameters

Sample	ΔG($kJmol^{-1}$)	ΔH($kJmol^{-1}$)	ΔS ($kJmol^{-1}K^{-1}$)
Blank	-	24.80	29.52
Piracetam	-13.03	55.53	44.6

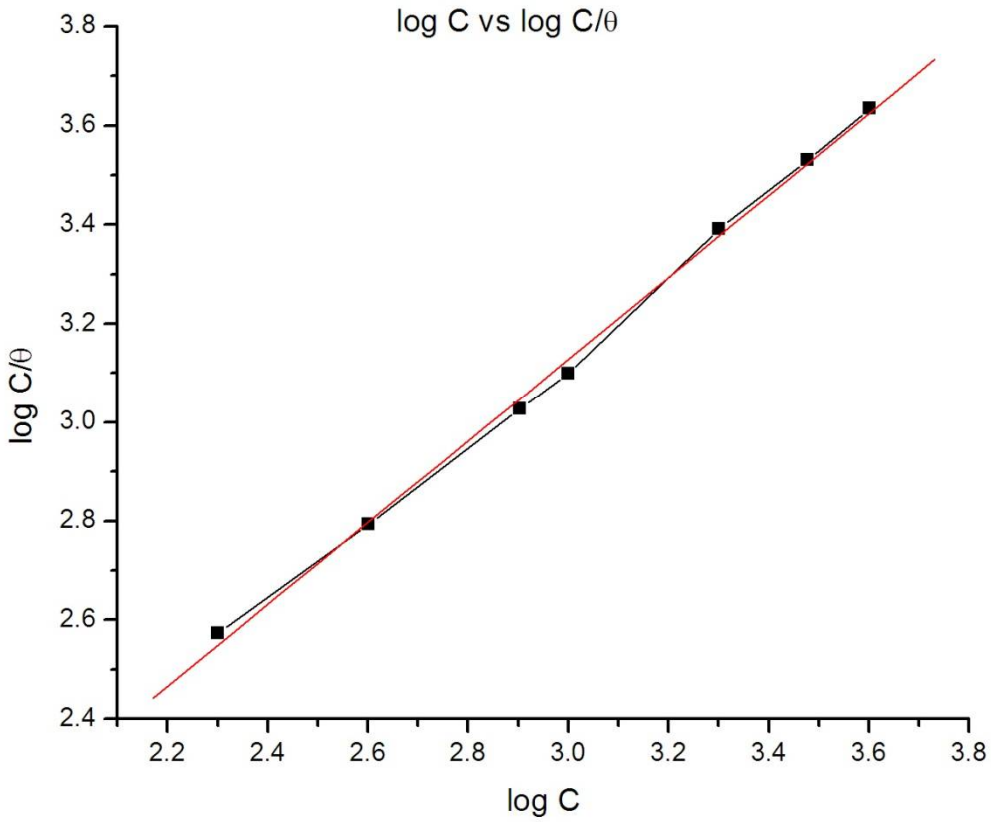


Figure14: log C vs. log C/surface coverage parameter

Scanning electron micropscopy: -

The surface morphologies of plain metal surface and metal in acidic solution and in the presence of Piracetam (4000 ppm)are shown in figures shown below. It is clear that the surface of plain metal before immersion displays a smooth surface. The metal coupon after immersion in acidic solution without the inhibitors demonstrated a rough and disintegrated surface due to corrosion, and the metal coupon immersed in a solution of 4000ppm along with acid shows visibly smooth surface with much less pores and cavities. This proves that Piracetam provides a protective covering on the metal surface thus, inhibiting corrosion. SEM analysis is done from IIT Roorkee.

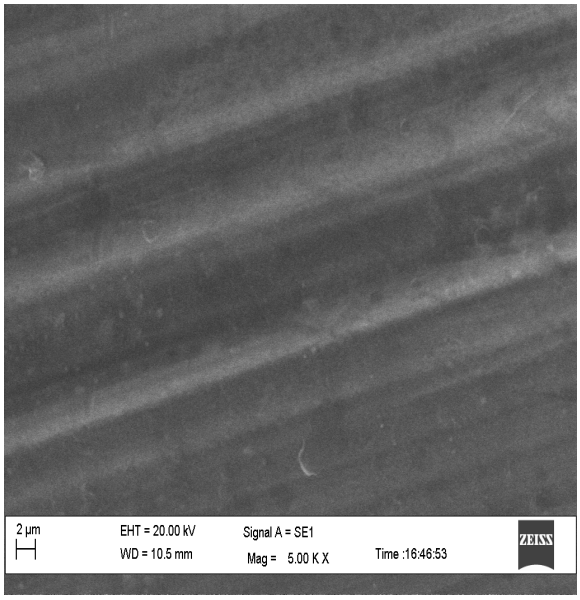


Figure 15: Plain Metal

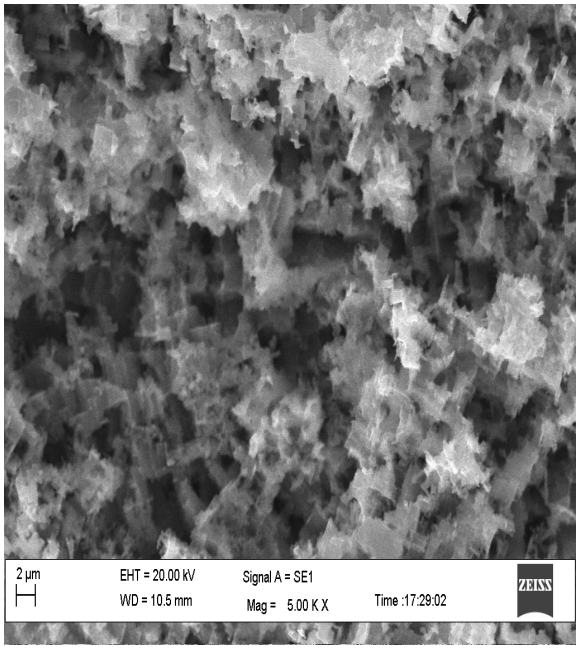


Figure 10: Metal Immersed In Acidic Medium

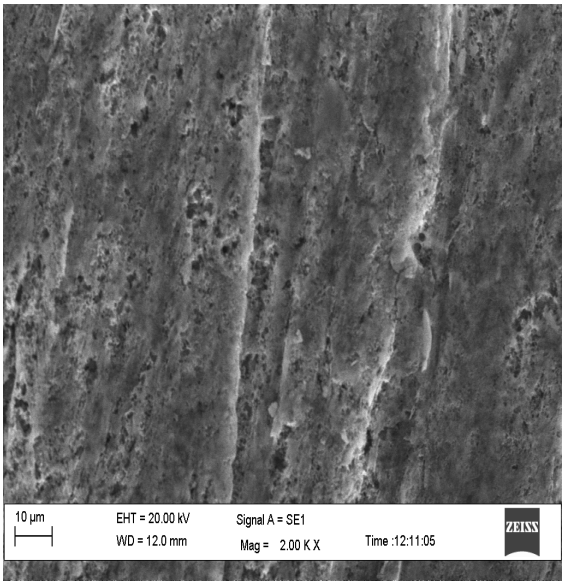


Figure 17: Metal with Inhibitor

AFM Analysis:- Atomic force microscopy is used to study the surface morphology of the metal. We have analysed three different metals a) plain metal b) metal in acidic medium c) metal with inhibitor. The results from AFM studies gives the average roughness of metal in these three cases and it has been observed that the plain metal is having low roughness parameter than metal in acidic medium but the metal with inhibitor have roughness parameter in between the two. It can clearly been said now that the decrease in roughness on metal surface after the addition of inhibitor. Hence, this is also satisfying the result and giving the agreement with all the data which has been quoted in this report. AFM provides the actual size, resolution and slope of the sample. Also, it gives the quantification of roughness of the sample. The main parameters is magnitude of roughness that is based on height distribution. AFM analysis is done from IIT Roorkee.

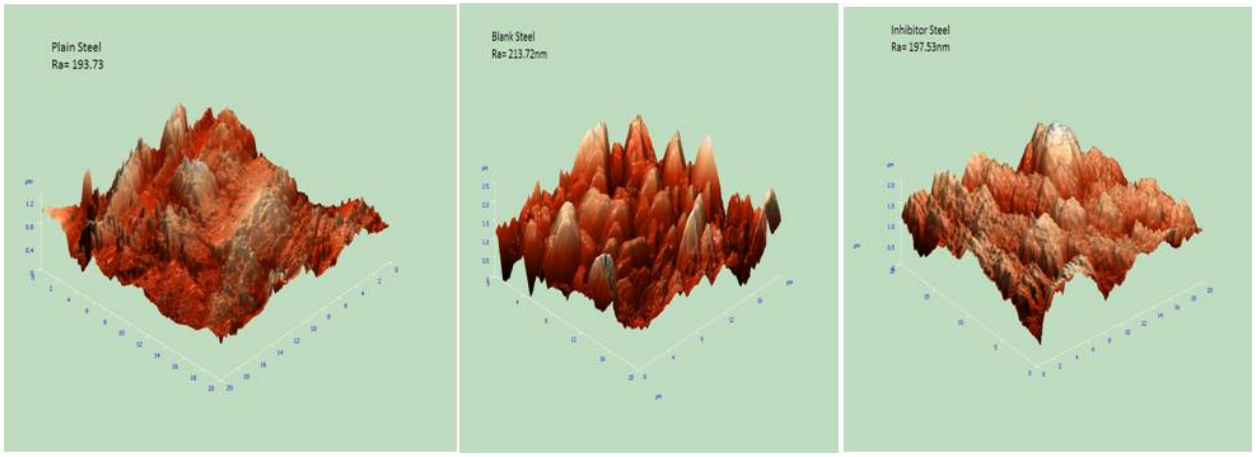


Figure 18: AFM data of Steel

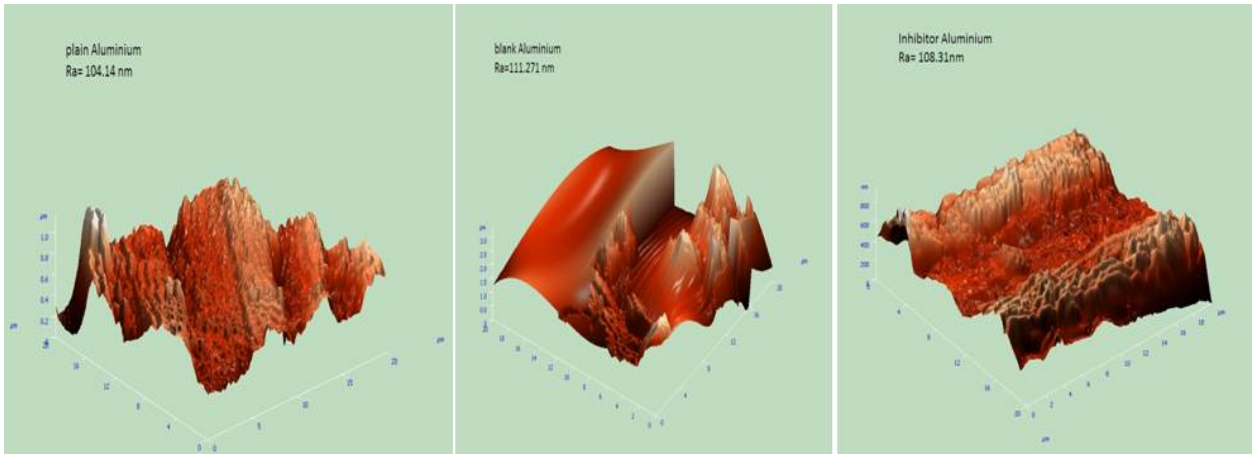


Figure19: AFM data of Aluminium

Potentiodynamic Polarization Studies: - The effect of Piracetam on the cathodic and anodic emmersion of mild steel in 7M H_2SO_4 varying the concentration of the inhibitor from 200 to 4000 ppm. Tafel slopes has been derived from the extrapolation of the data from the linear sections of cathodic and anodic sides. The elcetrochemical parameters like corrosion potential, current density and tafel plot of cathodic and anodic side. The relative inhibition efficiency is also calculated from these parameters and hence it has been concluded that Piracetam behave as both cathodic and anodic inhibitor(mixed-type of inhibitor). One more thing is clear from the data withdrwan from the polarization techniques is that when we increase the concentration of inhibitor the i_{corr} value is decreased from 200-4000ppm. The tafel plot of above discussion is shown below: -

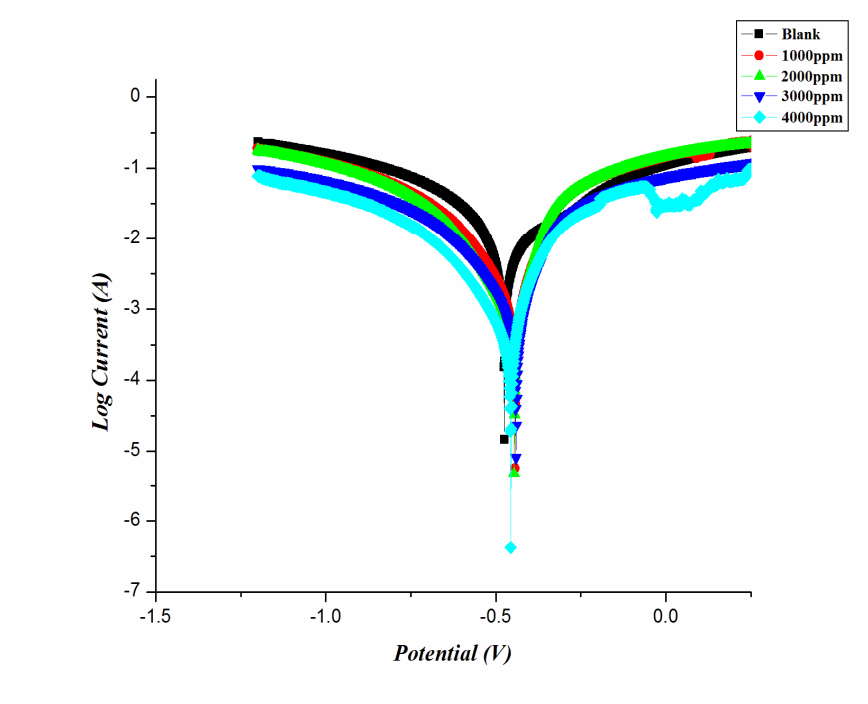


Figure20: Tafel Plot

This plot shows the relation between potential and current for mild steel in the presence of inhibitor and the table below shows the relative inhibitor efficiency and the anodic and cathodic values from tafel calculations.

Table 7: Tafel Calculations

Concentration	Icorr	$*10^{-3}$	IE	(-)Ecorr	Ba	Bc
1000	$1.26*10^{-3}$	1.26	83.9080	0.4430	11.2870	7.0700
2000	$0.823*10^{-3}$	0.823	89.4891	0.4460	11.970	7.8860
3000	$0.79*10^{-3}$	0.79	89.910	0.4410	10.2590	6.9990
4000	$0.537*10^{-3}$	0.537	93.1417	0.4560	9.9300	7.4200
blank	$7.87*10^{-3}$	7.83		0.4750	3.6000	5.8000

Electrochemical Impedance Spectroscopy: - The corrosion of mild steel in acidic solution with the presence of Piracetam was explored by EIS at 303 K after immersion for 3hrs. Two fold layer capacitance values (C_{dl}) and charge transfer resistance values (R_{ct}) got from impedance estimation. The estimation of charge transfer resistance was prevailed by measuring the width of the semicircle and the two fold layer capacitance. The graph for studies and the calculation table is given below.

Table 8: Electrochemical Impedance Studies

concentration	r_{ct} in	r_{ct} bl	f_{max} in	f_{max} bl	IE
1000	29.3400	13.9400	25.7000	9.7600	52.4880
2000	58.0200	13.9400	31.5000	9.7600	75.9738
3000	67.0100	13.9400	37.5000	9.7600	79.1971
4000	141.700	13.9400	42.0500	9.7600	90.1623

The value of R_{ct} increases in the presence of inhibitor which in turn leads to a decrease in corrosion current for mild steel in 7M H_2SO_4. All the concentrations of Piracetam performed good in acidic solution by enhancing the value of R_{ct} and bringing down the C_{dl} value. Higher values of R_{ct} in the presence of Piracetam as compared to R_{ct} value of blank are indicative of greater inhibition efficiency.

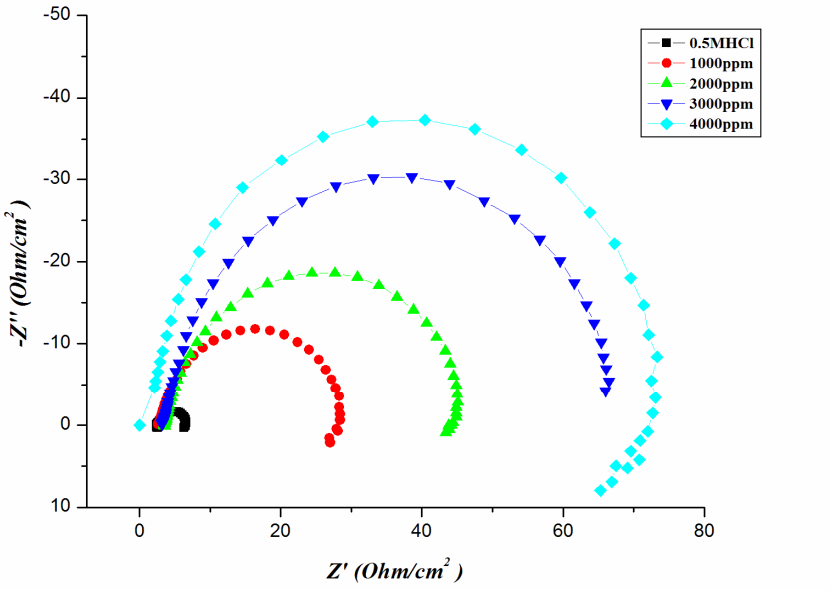


Figure21: Nyquist graph for mild steel with and without inhibitor in 7M H_2SO_4.

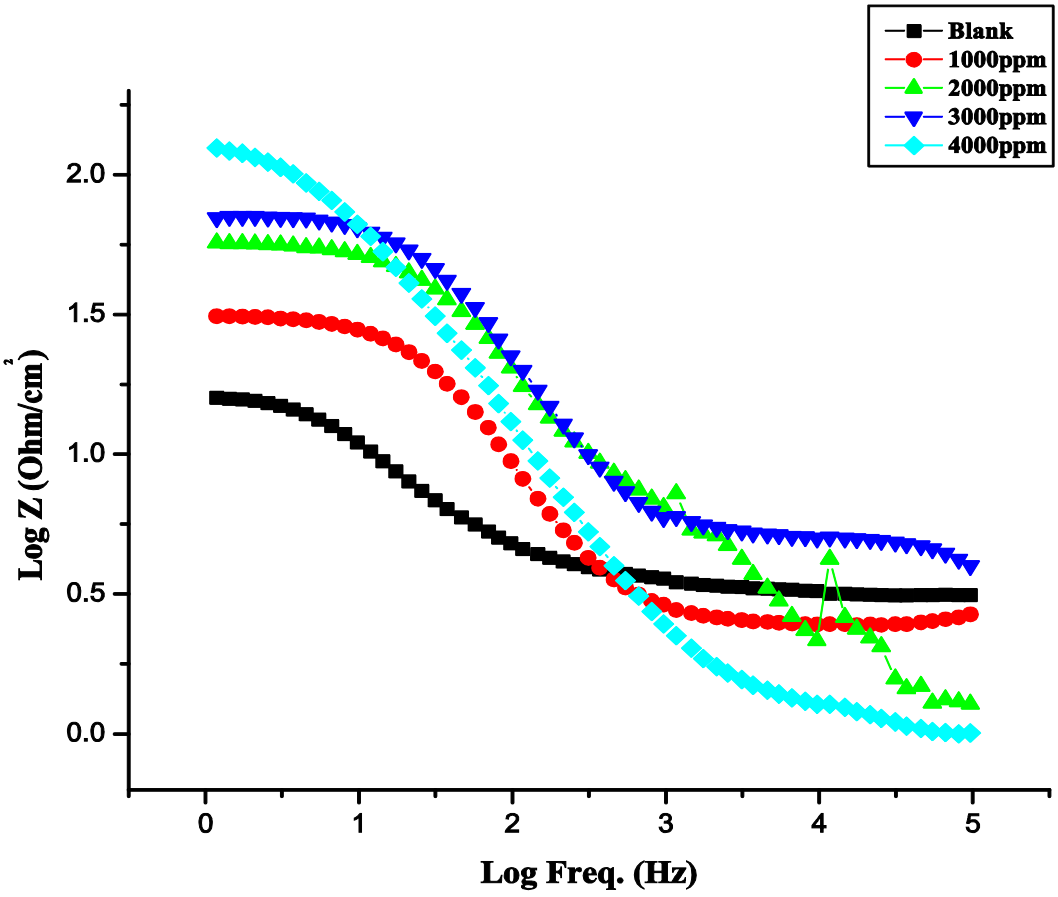


Figure 11: Bode Plot

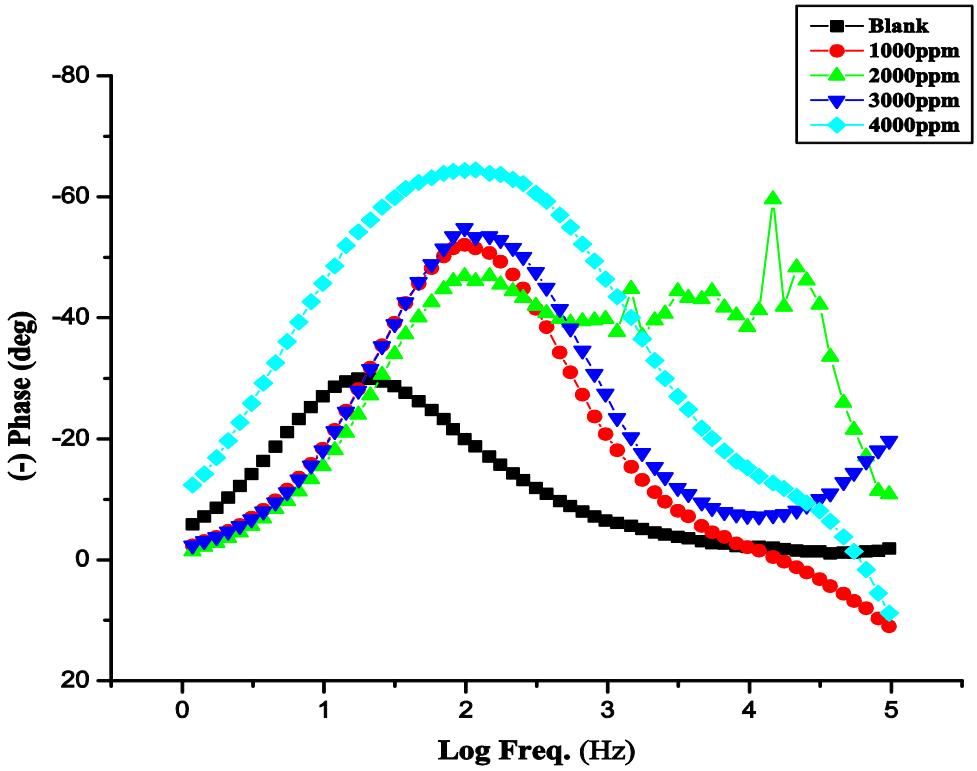


Figure 12: Bode Plot

Quantum chemical analysis: - The optimized structures, graphical surfaces of the highest occupied molecular orbital (HOMO) and possible sites for electrophilic attack are displayed in figures shown below. All quantum chemical parameters got from the optimized structures of lowest energy conformer. The reactivity of the Piracetam was concluded by investigating the frontier molecular orbital's. According to the frontier molecular orbital theory, chemical reactivity is strongly determined by the interaction of HOMO and the lowest unoccupied molecular orbital (LUMO) of the interacting species. The figures and the energy table is given below: -

Table 9: QCC

Type of inhibitors	E-HOMO	E-LUMO	ΔE
Piracetam	-5.80	--0.697	5.10

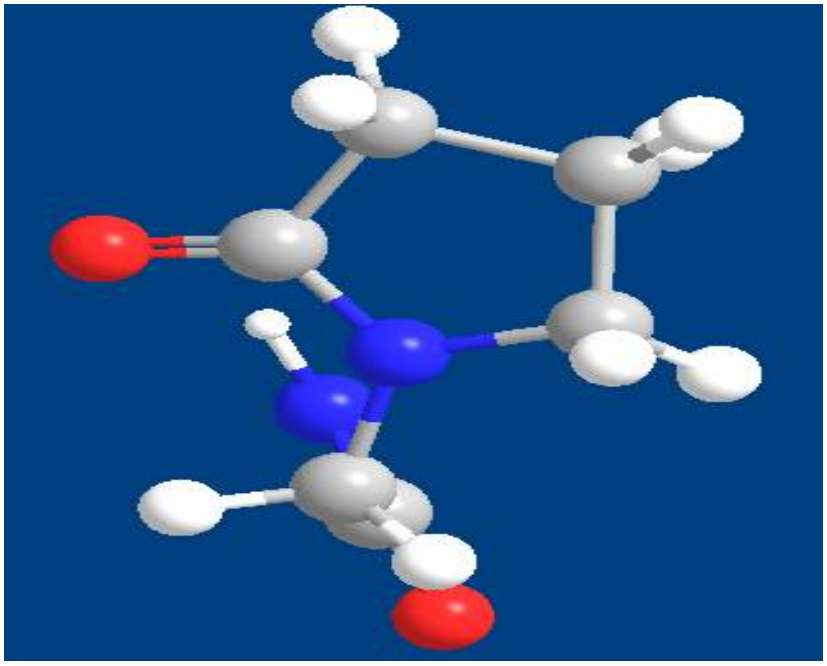


Figure22: Optimised structure of Piracetam

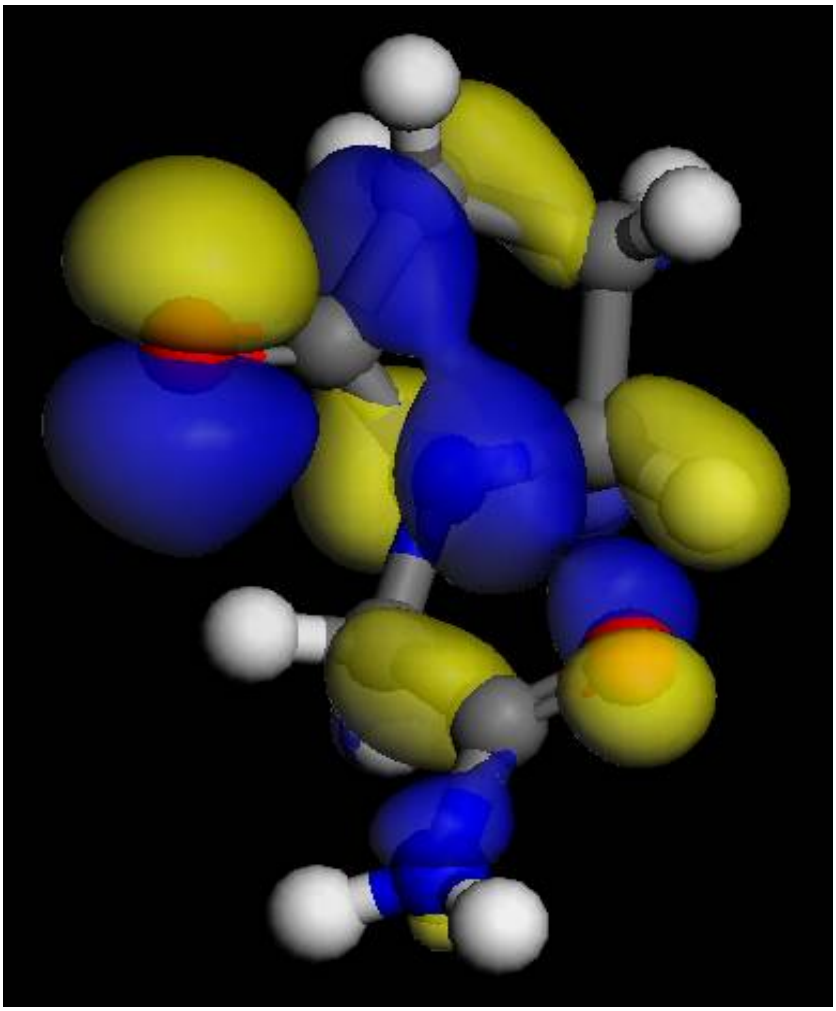


Figure23: HOMO of Piracetam

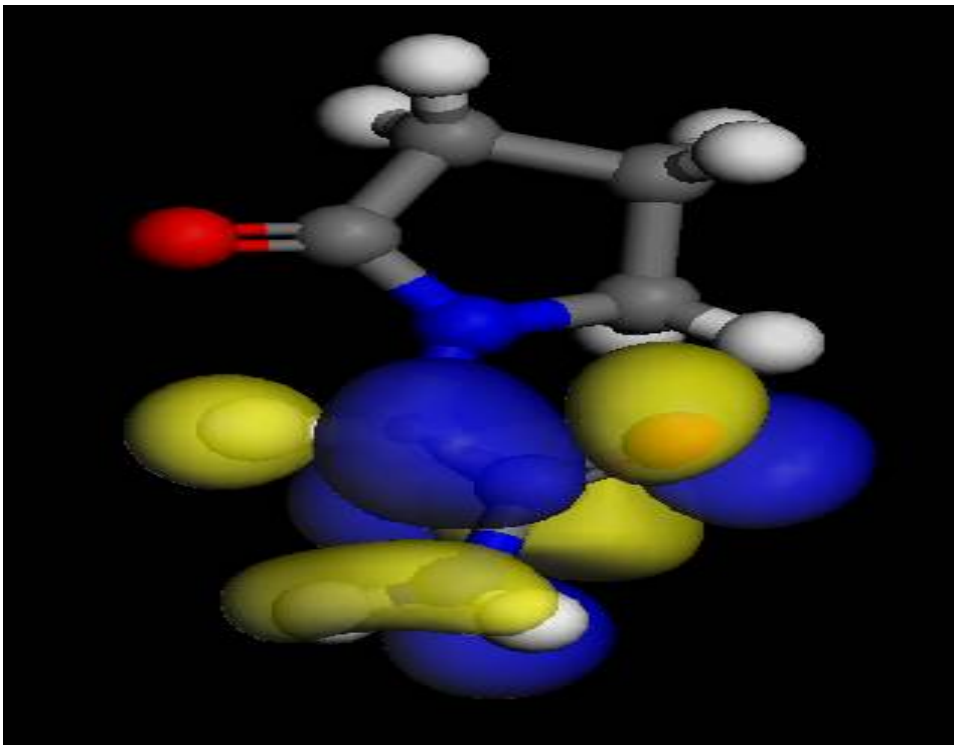


Figure24: LUMO for Piracetam

Montecarlo Studies:- Monte Carlo simulations using the Adsorption Locator and Forcite codes implemented in the Material Studio 6.0 software from Accelrys Inc. USA [1] was adopted to compute the adsorption energy of the interaction of Piracetam as inhibitor and a clean Fe and Al surfaces. For the whole simulation procedure, the Compass force field was used to optimize the structures of all components of the system of interest. The simulations were carried out in the simulation boxes (42Å× 42Å × 55Å) having α= 90.00o; β = 90.00o and γ = 90.00owith periodic boundary conditions in order to simulate a representative part of an interface devoid of any arbitrary boundary effects. The Fe(110) and Al(111) planes was next enlarged to a (10× 10) super cell. After that, a vacuum slab of 50Å thickness was built above the surfaces to convert the system to 3D periodicity. The optimized inhibitors using the Forcite code was then added near the surface of Fe(110) and Al(111)and a Monte Carlo simulation annealing procedure was carried out.

Table 10: MCC

Type of inhibitor	Total energy	Adsorption energy	Rigid adsorption energy	Deformation energy	Piracetam : dEad/dNi	H2O : dEad/dNi
Fe(110)/Piracetam/50H20	-560.61	-537.30	-562.00	24.70	-47.57	5.20

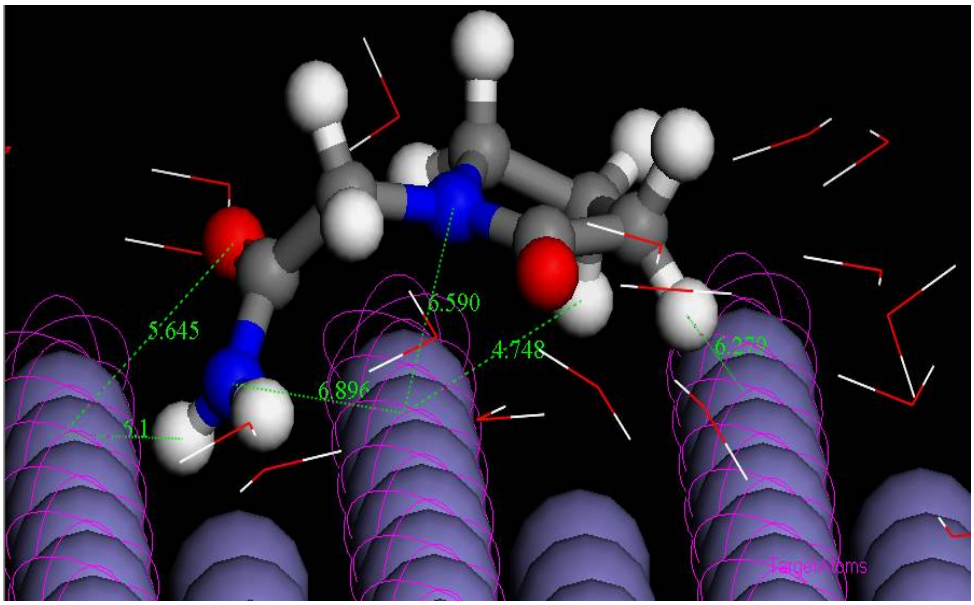


Figure25: The most stable low energy configuration for the adsorption of Piracetam on Fe(110)/50H2O system obtained using the Monte Carlo simulation, side view

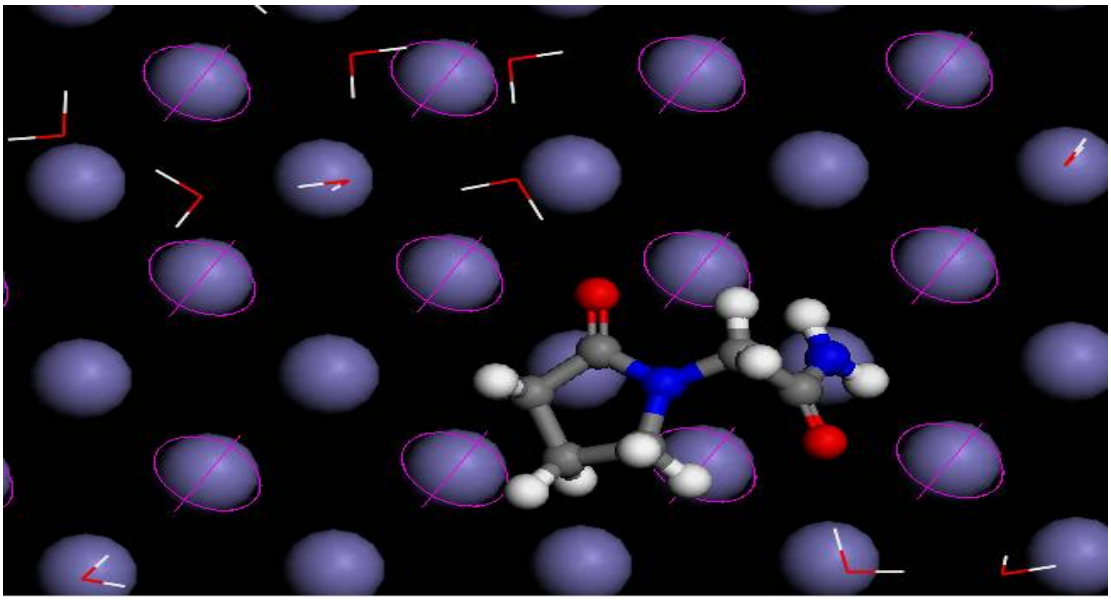


Figure26: The most stable low energy configuration for the adsorption of Piracetam on Fe(110)/50H2O system obtained using the Monte Carlo simulation, top view

Above table gives the monte-carlo simulation for mild steel in 7M H_2SO_4 in the presence of inhibitor. Electronic properties alone are not sufficient to see the pattern of the inhibition properties of inhibitor regardless of its accomplishment in investigating the mechanism of inhibitors. Along these lines, it is mandatory to display of the immediate collaboration of the inhibitors with mild steel within the presence of water to impersonate the genuine experimental condition. Monte Carlo technique is done to test possible low energy searches of the configuration space of the inhibitors on clean metal surface in aqueous solution as the temperature is steadily diminished.

The most stable low energy adsorption configurations of the inhibitor on Fe (III)/H_2O framework utilizing Monte Carlo studies. The qualities for the yields and descriptors of the Monte Carlo reenactments are recorded. It is very evident from the given table, which the adsorption energies of the inhibitors on Fe surface within the presence of water expanded. It is by and large recognized that the essential phenomenon of corrosion inhibition of Fe is by adsorption. So the adsorption energy can furnish us with immediate information about the efficiency of inhibitors.

In all cases, the adsorption energy of the Piracetam is far higher than that of water molecules This shows the likelihood of steady substitution of water molecules from the metal surface bringing about the formation of a protective layer which thereby inhibits corrosion on the surface of metal.

UV Analysis: - The UV is done with the help of SHIMADZU APPARATUS from Lovely Professional University. The samples are immersed for 24hrs the samples are then taken for the analysis. It had been found that the absorption of inhibitor is more than that of blank due to the transitions take place in inhibitor moiety. The transitions are from n to π^*. The increase in UV absorbance clearly depicting the efficiency of the metal. The transitions of metal are clearly shown in the graph shown below: -

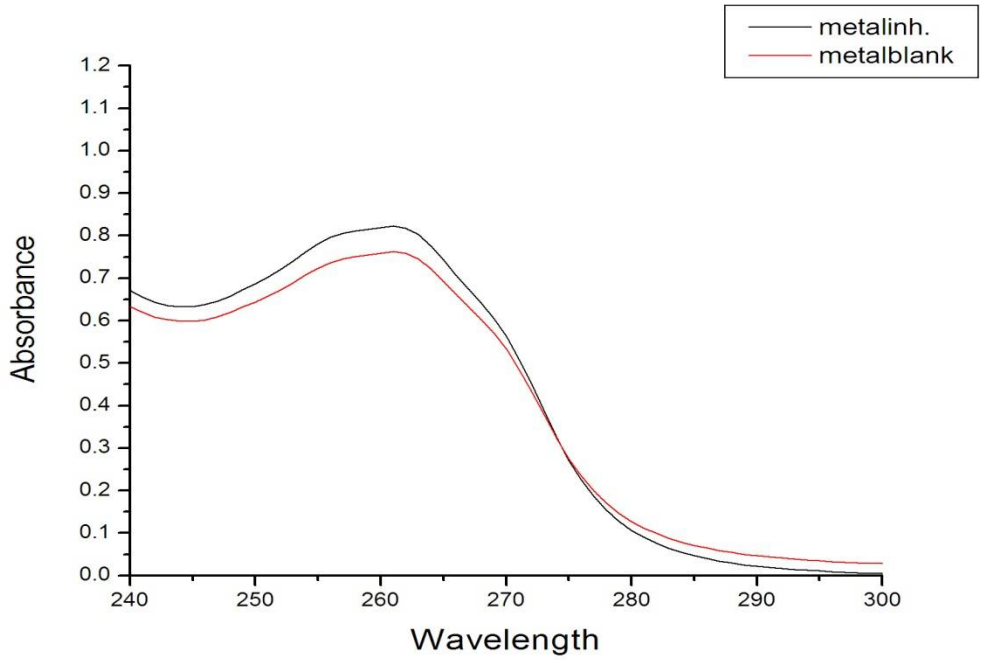


Figure27: UV Analysis Blank vs. Inhibitor

IR Analysis: -IR analysis is analyzed from SHIMADZU APPARATUS from LOVELY PROFESSIONAL UNIVERSITY. IR spectroscopy gives the difference in functional groups.

Here we compared the IR data of blank and that of inhibitor. In blank it is clear that there is no peak for CO stretch but in inhibitor we are getting all the possible peaks.

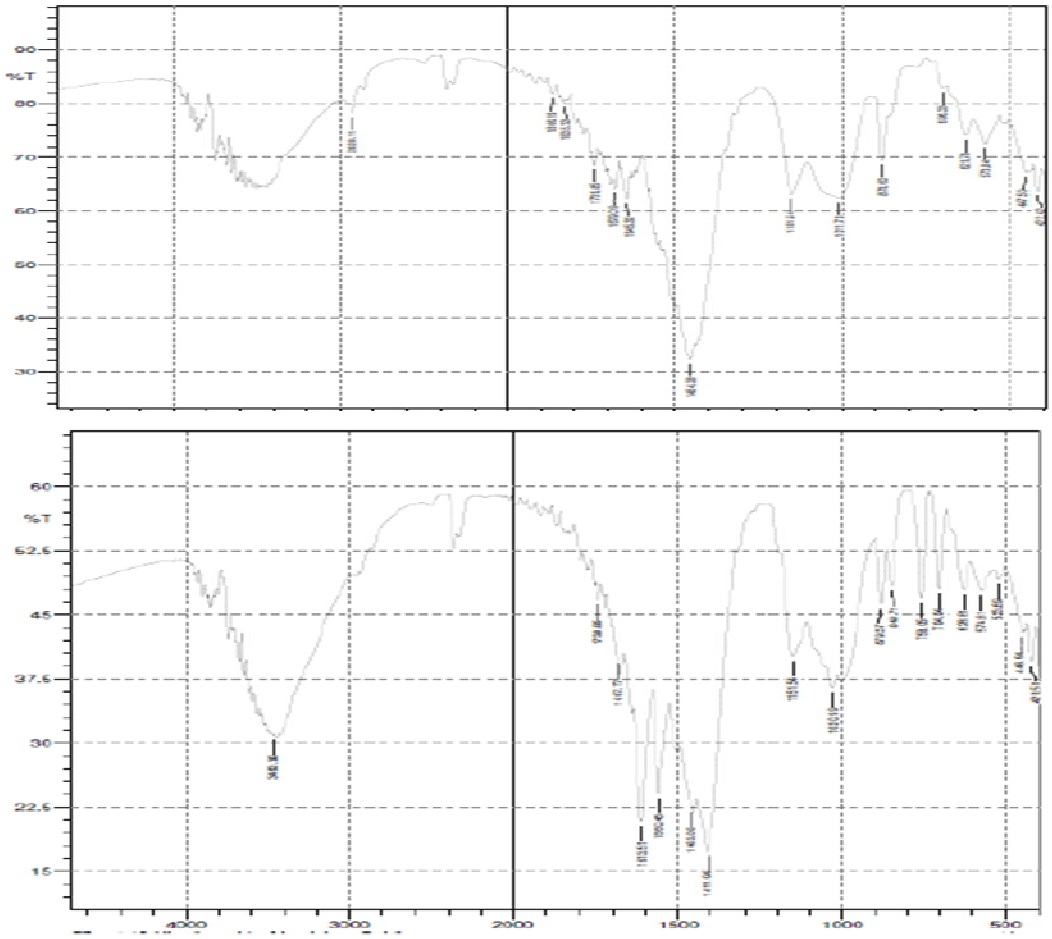


Figure28: IR analysis of Drug

Results and discussion for Aluminium:-

Weight loss studies:

Table 11: Acid Variation

concentration	Initial weight	final weight	Weight loss	%weight loss
0.1	0.3014	0.3013	0.0001	0.0331
0.15	0.3062	0.3060	0.0002	0.0653
0.3	0.3231	0.3180	0.0051	1.5784
0.35	0.2631	0.2208	0.0423	16.0775
0.5	0.3171	0.2589	0.0582	18.3538
0.55	0.2982	0.2209	0.0773	25.9221
0.7	0.2787	0.1873	0.0914	32.7951
0.75	0.3188	0.1763	0.1425	44.6988
0.9	0.2936	0.1463	0.1473	50.1702
0.95	0.3020	0.1245	0.1775	58.7748
1	0.3422	0.1274	0.2148	62.7703

The weight loss studies for aluminium are carried out in same way as that of steel. The metal is allowed to go through acid variation first and then a standard acid is chosen for further set of reactions. From the above table 0.75M is taken as the standard acid which gives ≈44% weight loss. The same set is repeated via taking Piracetam in the media and the results were like as follows:-

Table 12: Inhibitor Variation

concentration	Initial weight	Final weight	%weight loss	Inhibition efficiency
500	0.3056	0.2251	0.0805	48.0309
1000	0.3324	0.2603	0.0721	53.4538
1500	0.2785	0.2198	0.0587	62.1045
2000	0.2952	0.2481	0.0471	69.5932
2500	0.2745	0.2321	0.0424	72.6275
3000	0.3176	0.2802	0.0374	75.8553
4000	0.2904	0.2604	0.0300	80.6326
4500	0.2910	0.2658	0.0252	83.7314
5000	0.3112	0.2904	0.0208	86.5719
Blank	0.3392	0.1843	0.1549	0

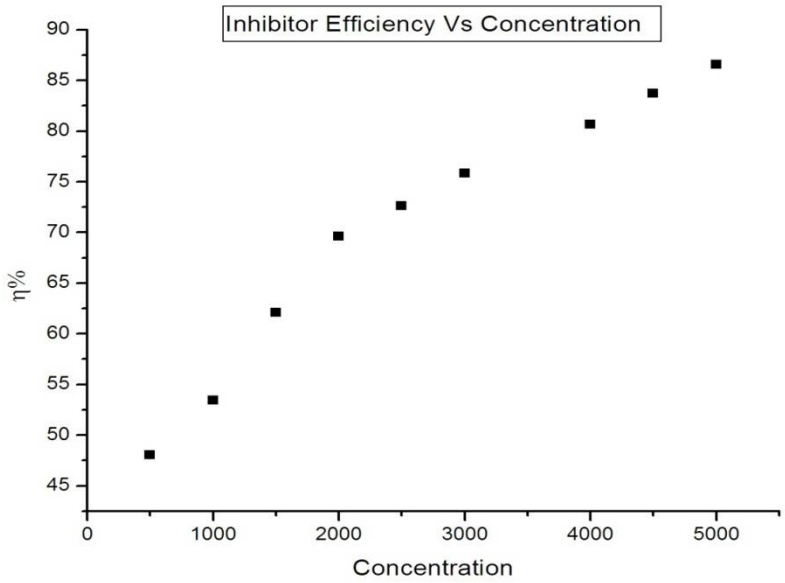


Figure29: Inhibitor Efficiency vs. Concentration

Effect of temperature:-

It is seen that with the increase in temperature the inhibition efficiency is decreased. The table of calculations is shown below.

Table 13: Temperature Variation

Temperature		Initial weight	Final weight	Wt. loss	%wt loss	Inhibition efficiency
25	Blank	0.3023	0.2704	0.0319	10.5524	
	Inhibitor	0.2915	0.2789	0.0126	4.3224	60.5015
30	Blank	0.2880	0.1593	0.1287	44.6875	
	Inhibitor	0.3164	0.2992	0.0172	5.4361	86.6355
35	Blank	0.3114	0.1462	0.1652	53.0507	
	Inhibitor	0.3007	0.2641	0.0366	12.1715	77.8450
40	Blank	0.3417	0.1002	0.2415	70.6760	
	Inhibitor	0.3113	0.2201	0.0912	29.2964	62.2360

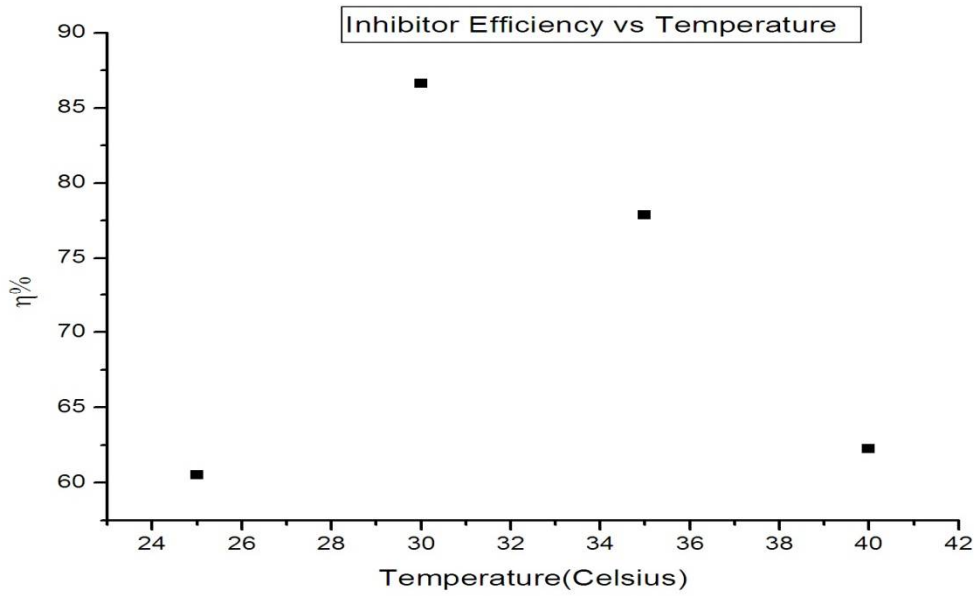


Figure30: Inhibitor Efficiency vs. Temperature

Time Variation: - With increase in duration of time the inhibition efficiency show the gradual increase in the trend.

Table 14: Time Variation

Time		Initial weight	Final weight	Wt. loss	%wt loss	Inhibition efficiency
20	blank	0.3072	0.1872	0.1200	39.0625	
	inhibitor	0.3018	0.2520	0.0498	16.5009	58.5000
40	blank	0.3267	0.1908	0.1359	41.5977	
	inhibitor	0.2740	0.2343	0.0397	14.4890	70.7873
60	blank	0.3245	0.1807	0.1438	44.3143	
	inhibitor	0.3103	0.2897	0.0206	6.6387	85.6745
80	blank	0.3159	0.1486	0.1673	52.9597	
	inhibitor	0.3311	0.3165	0.0146	4.4095	91.2731

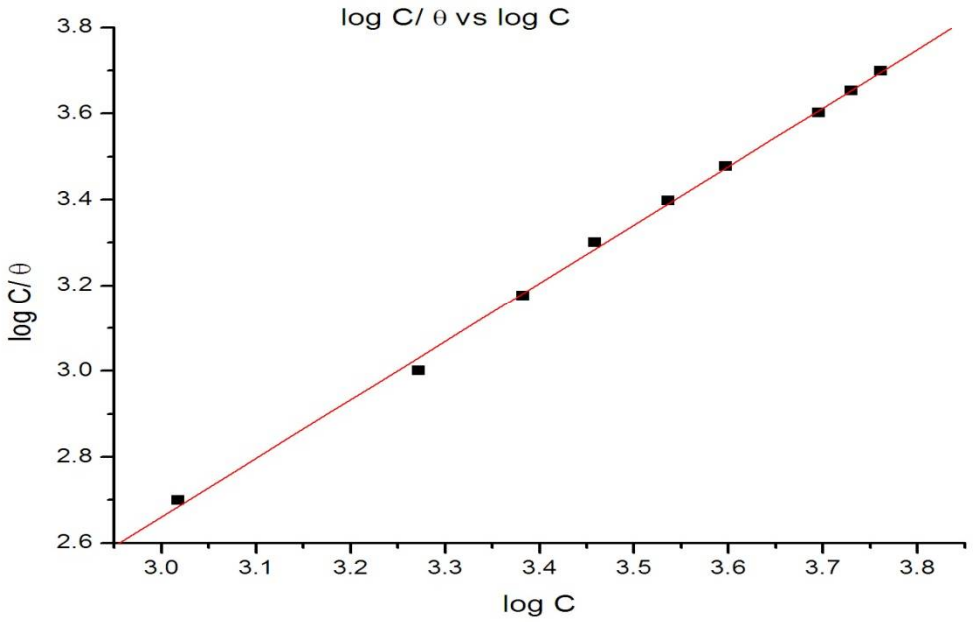


Figure31: Langmuir Isotherm

Slope ≈ 1

The slope of above variation is almost equal to 1, which indicates that the Langmuir adsorption isotherm is obeyed for the adsorption of Piracetam on the surface of the metal. The graph itself shows the linearity in the trend.

Arrhenius equation is used to calculate the activation energy of the process: -

$$C_R = A \exp(-Ea/RT)$$

The symbols have their usual meanings.

A - Arrhenius Equation

E_a – Activation Energy

C_R- Corrosion Rate

R- Rate Constant

T- Temperature

Table 15: Activation Energy Parameters

Sample	E_a(kJ/mol)	ΔH(kJ/mol)	ΔS($kJmol^{-1}K^{-1}$)
Blank	15.72	6.97	7.20
Piracetam	30.30	26.42	19.75

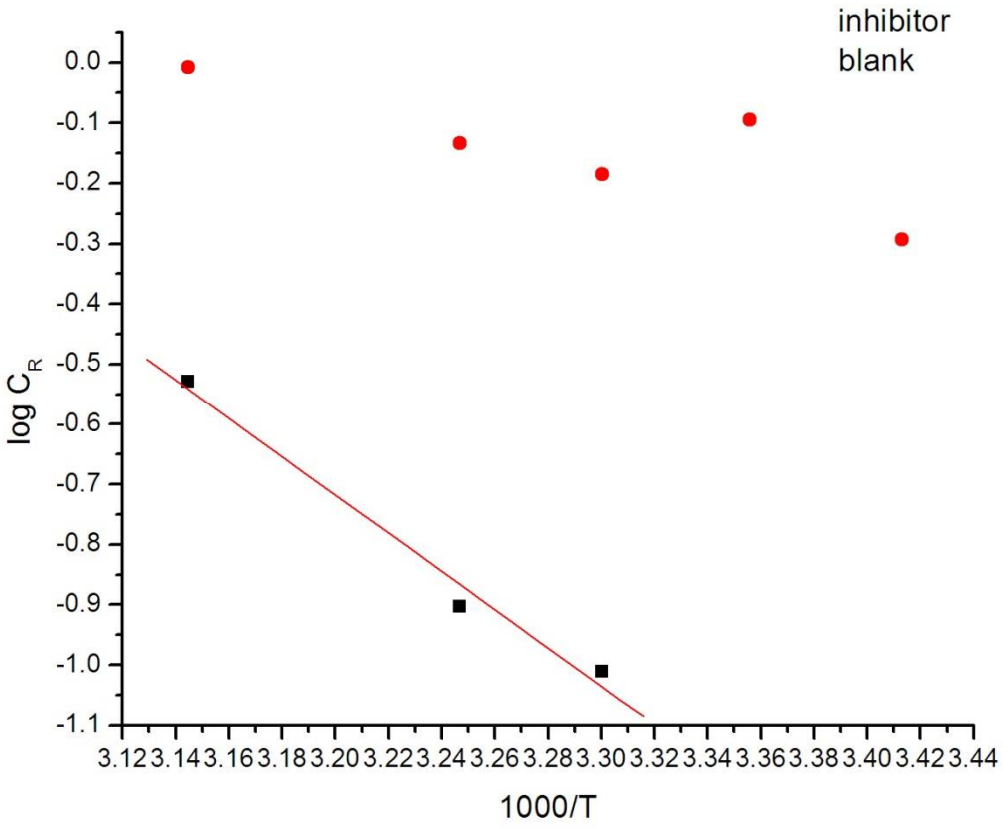


Figure32: Activation Energy

Thermodynamics studies: - The data obtained from thermodynamics parameters plays a very important role in deciding the role of inhibitor effective for corrosion studies. Various parameters like gibb's free energy, entropy, enthalpy and heat of adsorption. The formula used for calculating the gibbs free energy is as follows: -

$$\Delta G^0_{ads} = -2.303RTlog(55.5Kads)$$

where, T is the temperature of the system and the constant value 55.5 is the molar concentration of water. To get spontaneos reaction the value of ΔG should come out to be negative. The ΔG is

coming out to be -13.086 $kJmol^{-1}$ for inhibitor which explains the electrostatic interaction between the charged metal surface and the charged organic molecules present in the drug. From the equation: -

$$lnkads = -(\Delta H^0_{ads}/RT) + C$$

It is clear that ($\Delta H_{ads}/R$) gives the slope of the equation when the graph is plotted between ln K_{ads} vs. 1000/T. the graph comes out to be straight line and the slope gives the respective values. In the equation, R is the universal gas constant, T is temperature of the system, ΔH_{ads} is the heat of enthalpy of the system.

Table 16: Thermodynamic Parameters

Sample	ΔG($kJmol^{-1}$)	ΔH($kJmol^{-1}$)	ΔS ($kJmol^{-1}K^{-1}$)
Blank	-	6.97	7.20
Piracetam	-21.03	26.42	19.75

Conclusions

- Weight loss studies showed that piracetam acts as an efficient corrosion inhibitor with maximum efficiency being 93% at 4000ppm concentration of inhibitor.
- The inhibition efficiency increases with increase in concentration of inhibitor and decreases with increase in temperature.
- Electrochemical measurements were in good agreement with weight loss studies and tafel studies showed that piracetam acted as a mixed type of inhibitor,.
- The mechanism of corrosion inhibition was seen to be physical adsorption and it followed Langmuir adsorption isotherm.
- Theoretical studies were done by quantum chemical studies and Montecarlo simulation studies. The parameters calculated include EHOMO, ELUMO, ELUMO-EHOMO, dipole moment etc.
- The results from weight loss studies, electrochemical studies and the theoretical studies are in good agreement with each other.

It has been observed from the experimental data and the results from them that Piracetam is a good corrosion inhibitor for both mild steel and aluminium and in the cases it shows its highest efficiency up to the average of ≈93%. This is a good number for a drug that can also behave as a good corrosion inhibitor and is cost effective. The experimental work or the weight loss studies shows the very good agreement with the theoretical studies includes Quantum Chemical Calculations and Montecarlo simulations.

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