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A STUDY OF RAPE-CAKE EXTRACT AS ECO-FRIENDLY VAPOR PHASE CORROSION INHIBITOR

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Abstract. Rape-cake extract was developed as novel volatile corrosion inhibitors. Its volatiles were analysed by GC-MS. A semi empirical approach was used to rationalize the rape-cake extract inhibitory action. The molecular spatial structure, energy gap and density of extract main compounds have been theoretically investigated using HyperChem7.00.

Keywords: rape-cake extract, volatile corrosion inhibitor, DFT calculation.

1. Introduction

Atmospheric corrosion of metals in closed spaces, such as in parcels, and during storage and shipment, can be temporarily prevented by the use of certain substances called vapour phase corrosion inhibitors. A vapour phase corrosion inhibitor (VPI) is a compound that has the ability to vaporize and condense on a metallic surface to make it less susceptible to corrosion. The main advantage of VPIs compared with conventional corrosion control methods stems from their gas-phase transport. A VPI reaches the metallic surfaces without contacting the surface directly. The efficacy, convenience, and cost effectiveness of VPIs made their application for rust control almost universal in automotive-manufacturing, steel-making, ship-building, power generation, and defence production [1].

It was found that certain specific VPI formulations can in fact be toxic. For example, dicyclohexyl ammonium nitrite (DICHAN) has been found to be the most effective for inhibiting the atmospheric corrosion of steel, and gained industrial application for several decades [2]. Research confirmed that some N-nitrosoamines, including those generated by DICHAN, were not only carcinogenic, but also hemotoxic as well. Most of the volatile corrosion inhibitors are synthetic chemicals, expensive, and very hazardous to environments. Thus, an alternative of environmental-friendly VPIs is under consideration [3-6].

Nowadays, natural products are viewed as incredibly rich sources of naturally synthesized chemicals for use in most applications. Some of the advantages that natural chemicals have over other types of chemicals include their environmental acceptability and availability. Plant extracts are environment friendly, bio-degradable, non-toxic, easily available and of potentially low cost. Most of the naturally occurring substances are safe and can be extracted by simple procedures. Recent literature is full of researches which test different extracts for corrosion inhibition applications. Numerous naturally occurring products such as *Prosopis juliflora* [7], *Eugenia jambolans* [8], *Lawsonia opuntia* [9], *Swertia aungustifolia* [10], *Ficus religeosa* [11], *heena* [12], *Datura stromonium* [13] and *calotropis* plant extracts have been evaluated as potential corrosion inhibitors.

Many of these naturally occurring substances proved their ability to act as corrosion inhibitors for the corrosion of different metals and alloys in different aggressive media. Despite that many plant extract have not been studied as volatile corrosion inhibitors. The rape-cake extract (*Brassicaceae*), which contains many chemicals compounds, may be used as VCIs. Hence, in the present work it has been aimed to investigate the corrosion inhibition efficiency of rape-cake extract as volatile corrosion inhibitors for mild steel.

2. Experimental

2.1. Materials and Apparatus

The corrosion test and electrochemical measurements were carried out using mild steel strips. The composition of the mild steel is given in %: C 60.15; Mn 0.20–0.45; P 60.03; S 60.035 and Al, P 0.02. Steel specimens (50×20×1.5 mm) were used for volatile

inhibiting sieve test (VIS). The strips were polished by emery paper of 1/0, 2/0 and 3/0 rinsed with double distilled water, degreased and dried at room temperature.

Rape-cake extract was prepared by macerating in the 2-propanol alcohol for 48 h and filtered through ordinary filter paper.

2.2. Gravimetric Measurements

Volatile inhibiting sieve tests were applied to evaluate the inhibition effect of the VCIs. To obtain reproducible results three samples were used in each test simultaneously. There was a hole in each plate drilled to suspend the sample by a nylon thread. The samples were grinded with SiC paper to 1000 mesh and were then cleaned in alcohol and rinsed before drying at room temperature. The final geometrical area was 25 cm^2. The gravimetric measurement was conducted by suspending the samples in a 250 cm^3 conical flask with a tight-fitting rubber cork containing a small dish. The VCIs were dispersed in the dish. The samples with freshly prepared surface were mounted on the flask with and without 1.0 g inhibitor, respectively. After inhibitor film-forming period of 3 days, 15 cm^3 deionized water was added. The test process included cyclic warming and cooling of the samples in a corrosion testing chamber of varying humidity. One cycle included an 8 h exposure in the thermostat (323 ± 1 K), and 16 h exposure at room temperature. The duration of the test was 21 days.

Corrosion rates *CR* (g·m^{-2}·h^{-1}) and inhibitor effectiveness *IE* are calculated by means of the following equations:

$$CR = \frac{W_0 - W_1}{A \cdot T} \qquad (1)$$

where *A* is the sample area, m^2; W_0 is initial weight of the sample, g; W_1 is sample weight after the immersion period, g; *T* is the immersion period (in h), and CR_1 and CR_2 are the corrosion rates without and with inhibitor, respectively.

$$IE = \frac{CR_1 - CR_2}{CR_1} \cdot 100 \qquad (2)$$

2.3. Electrochemical Measurements

Electrochemical measurements were carried out in stimulated atmospheric corrosion solution in a three-electrode cell, consisting of a mild steel rod working electrode (WE), a platinum foil counter electrode (CE), and a saturated calomel electrode (SCE) as reference electrode. Polarization electrochemical studies were performed at the facility which includes potentiostat PI-50-1 and programmer PR-8. Since it is known that the cathodic process of atmospheric corrosion occurs mainly

with oxygen depolarization and great speed, the electrochemical study was conducted under stirring for uniform oxygen flow to the metal surface electrode. We use the mixer MM-5. The WE was mechanically polished on wet silicon carbide (SiC) paper, rinsed with double-distilled water, degreased with acetone and ethanol, and dried at room temperature. The WE was embedded into an epoxy resin holder exposing 0.385 cm^2 surfaces to the solution.

The potential values reported here were versus SCE. The cell was open to the laboratory air and the measurement was conducted without agitation at room temperature (298 K). All the experiments were carried out in 1N Na$_2$SO$_4$ solution as electrolyte. *IE* of potentiodynamic polarization measurement was defined as:

$$IE = \frac{I_{corr} - I_{corr(ing)}}{I_{corr}} \cdot 100 \qquad (3)$$

θ represents the surface coverage calculated by the following relationship:

$$q = \frac{I_{corr} - I_{corr(ing)}}{I_{corr}} \qquad (4)$$

where I_{corr} and $I_{corr(inh)}$ are the uninhibited and inhibited corrosion current density values.

2.4. SEM Analyses

The surface morphology and coating were examined by FEI E-SEM XL 30.

2.5. GC-MS Analysis

Component composition of volatile rape-cake extract was investigated by gas chromatography-mass spectrometry on a gas chromatograph "FINIGAN FOCUS" as a detector with a gas chromatograph. For separation of volatiles the 30 m, 30.25 mm I.D., $d_f = 0.25$ μm fused-silica column (HP-5 MS, Hewlett-Packard) was used. The injector and detector temperatures were 523 and 553 K, respectively. Helium was used as carrier gas. The column oven was programmed from 373 K→ 10 K/min → 553 K. The temperature of the GC-MS transfer line was 553 K. The mass spectral identification of the free and bound aromatic compounds was carried out by comparing to the NIST-5 (National Institute of Standards and Technology, Gaithersburg, MD). Qualitative analysis (mass spectral data) was verified by comparing the retention indices and mass spectra of identified compounds with those of authentic reference substances.

2.6. Quantum Chemical Calculations

Quantum chemical calculations have been performed by the HyperChem 7 [14] package. The

geometry optimization was obtained by application of the restricted Hartree-Fock method (RHF) using MNDO approach with PM3 parameterization.

According to Koopman's theorem, the frontier orbital energies E_{HOMO} and E_{LUMO} are related to the ionization potential I, and the electron affinity A of iron and the inhibitor molecule by the following relations: $A = -E_{LUMO}$, $I = -E_{HOMO}$. Absolute electronegativity χ and absolute hardness η of iron and the inhibitor molecule are given by [15]:

$$c = \frac{1}{2}(I + A) \qquad (5)$$

$$h = \frac{1}{2}(I - A) \qquad (6)$$

The softness σ of the inhibitor molecule is simply the inverse of the hardness: $\sigma = 1/\eta$.

If bulk iron metal and the inhibitor molecule are brought together, the flow of electrons will occur from the molecule of lower electronegativity to the iron that has higher electronegativity until the value of the chemical potential becomes equal. The fraction of electrons transferred from the inhibitor molecule to the iron atom will then be given by Eq. (7) [15]:

$$\Delta N = \frac{c_A - c_B}{h_A + h_B} \qquad (7)$$

where a theoretical value of $\chi Fe \approx 7$ eV [16] is taken for iron and $\eta_{Fe} = 0$ is taken assuming that $I = A$ for bulk metals [17].

3. Results and Discussion

3.1. Inhibition of Mild Steel Corrosion by the Film of Rape-Cake Extract

The corrosion rate and inhibition efficiency of mild steel in environment at 100 % RH in the absence and presence of rape-cake extract are given in Fig. 1. The increase of extract concentration decreases the corrosion rate. The inhibition efficiency achieves 94 %. This shows that rape-cake extract can be volatilized and adsorbed on the mild steel surface to protect the steel. To provide high protection the minimal v/v ratio inhibitor : enclosed space equal to 1:100 is sufficient.

3.2. Electrochemical Measurements in Stimulated Atmospheric Corrosion Solution

Potentiodynamic polarization curves for mild steel in 1 N Na_2SO_4 are shown in Fig. 2. As one can see, the inhibitor causes a decrease in the corrosion rate, *i.e.* shifts

the anodic curves to positive potentials. It is also seen that all these samples shift the corrosion potential significantly to noble direction therefore they are predominantly anodic inhibitors. The inhibition efficiency increases as the extract concentration is increased.
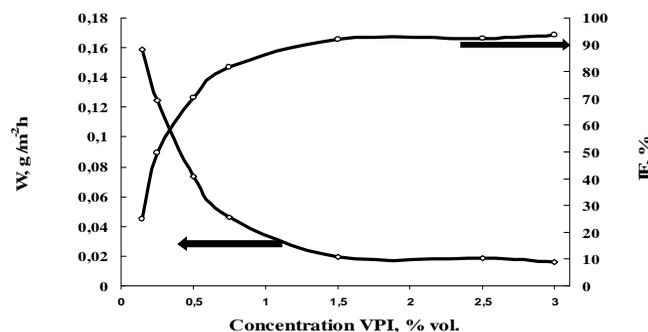

Fig. 1. Variation of corrosion rate (*CR*) and inhibition efficiency (*IE*) of corrosion of mild steel for volatile corrosion inhibition test
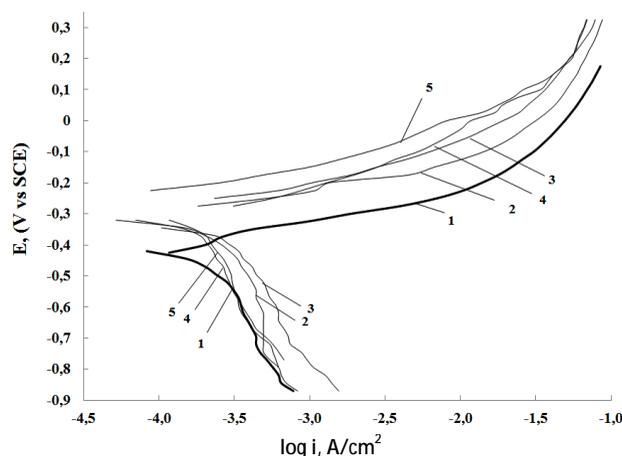

Fig. 2. The polarization behaviour of mild steel in 1 N Na_2SO_4 with (2-5) and without film (1) obtained after the formation for 48 h in the vapour phase of rape-cake extract at the v/v ratio of inhibitor: enclosed space (100 ml): 0.1 (2); 0.75 (3); 1.0 (4) and 2.5 (5)

3.3. Adsorption Isotherm

It is generally accepted that organic molecules inhibit corrosion by adsorption at the metal surface and the adsorption depends on the molecule's chemical composition. Basic information on the adsorption of inhibitor on metals surface can be provided by adsorption isotherm. Adsorption isotherm plot surface coverage (θ) obtained from polarization measurements versus log concentration (vol %) are shown in Fig. 3. Inhibitor concentration was varied in the range of 0.15–5 vol %.

The straight lines of these plots suggest that the adsorption of volatile compound of the rape-cake extract on mild steel obeys Langmuir adsorption isotherm.
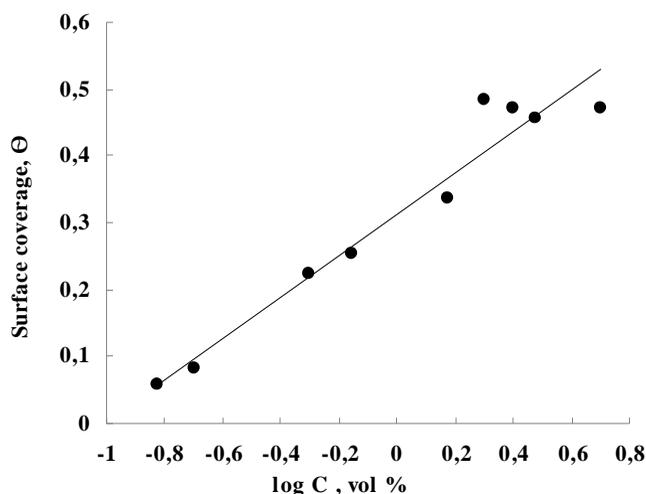

Fig. 3. Langmuir adsorption isotherm plot for mild steel in 1N Na_2SO_4 after the film-forming of rape-cake extract

3.4. SEM Analyses

SEM analyses were conducted in order to characterize the protective layer that formed on the low carbon steel surface. SEM images initial surface and after 48 h for VCI film-forming are shown in Fig. 4.

The surface morphology of the sample before exposure to volatiles of extract indicates there were a few scratches from the mechanical polishing treatment. This image displays a freshly polished steel surface. The following image (Fig. 4b) is of the steel surface after 48 h of exposure for the film-forming of the rape-cake extract. It shows a thin and covering surface film.
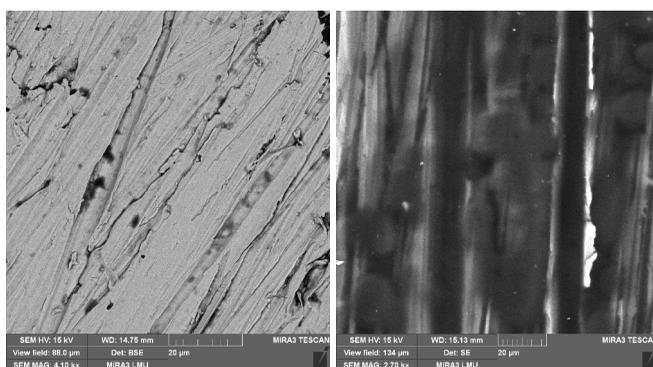

a)   b)

Fig. 4. SEM images of the carbon steel surface: initial surface (a); after 48 h exposure for VCI film-forming (b)

3.5. Analysis of Volatiles in Rape-Cake Extract by Gas Chromatography-Mass Spectrometry

The volatile chemical composition of rape-cake extract is highly complex containing glycosides, nucleosides, ketone, aldehyde, saturated and unsaturated fatty acids, sterols, and alkaloids (Table 1). The most abundant compounds were guanosine (about 10 %), xanthosine (8 %), dimethoxyacetophenone (12 %), benzaldehyde, 4-hydroxy-3,5-dimethoxy (11.5 %), as well as oleic, linoleic and palmitic acids (about 32 %).

Table 1

**The content of the main components
of 2-propanol rape-cake extract**

Name of the component	Weight ratio, %
Guanosine	10.4
Sucrose	6.2
Xanthosine	8.3
3',5'-Dimethoxyacetophenone	12.3
Benzaldehyde, 4-hydroxy-35-dimethoxy	11.5
Acetic acid	5.6
n-Cyclohexyl-4-hydroxybytyramide	1.6
Palmitic acid	6.1
Linoleic acid	9.8
Oleic acid	10.2
Pyrrolidine, 1-(1-oxo-7,10-hexadecadienyl)	1.5
2-Pyrrolidine, 1-(9-octadecenly)-	1.2
Ethanamine, 2,2'-oxybis[N,N-dimethyl]-	4.5
7-Dehydrodiosgenin	1.4
Campesterol	1.9
γ- Sitosterol	1.1
b-Sitosterol	2.9
Ergosta-5,22-dien-3-ol	1.7
Stigmast-4-en-3-one	0.9
Stigmast-3,5-dien-7-one	0.8

The inhibition of mild steel corrosion by rape-cake extract is probably attributed to the presence of glycosides, keton and aldehyde since these compounds contain such centres of adsorption as oxygen and nitrogen atoms. All individual chemical compounds are known as inhibitors for several metals [18, 19]. However, it remains unknown what molecules of vapour-phase rape-cake extract are adsorbed on the steel surface and provides inhibition effectiveness.

Studies report that the adsorption process depends on the physicochemical properties of inhibitor molecule, related to the electronic density of donor atoms and on the possible steric effects. It has been established that

corrosion inhibitors usually promote the formation of a chelate on the metal surface, which include the transfer of electrons from the organic compounds to the metal, forming a donor-acceptor bond during the chemical adsorption process [20-28]. In this adsorption, the metal acts as an electrophile while the inhibitor acts as a nucleophile [29]. Considering the charge transfer characteristics of the adsorption, the wide use of quantum chemical calculations to study this process is justified [30]. Thus, adsorption power of molecules of vapour-

phase rape-cake extract was investigated using quantum chemical concepts and the density functional theory (DFT) was applied to study the geometrical and electronic structures of the extract compounds.

The inhibitor molecules structure of rape-cake extract obtained after a geometric optimization procedure using HyperChem 7.0 computer package (RHF calculation, singlet state, PM3 parameterization) and density of the highest occupied molecular orbital are given in Figs. 5 and 6.
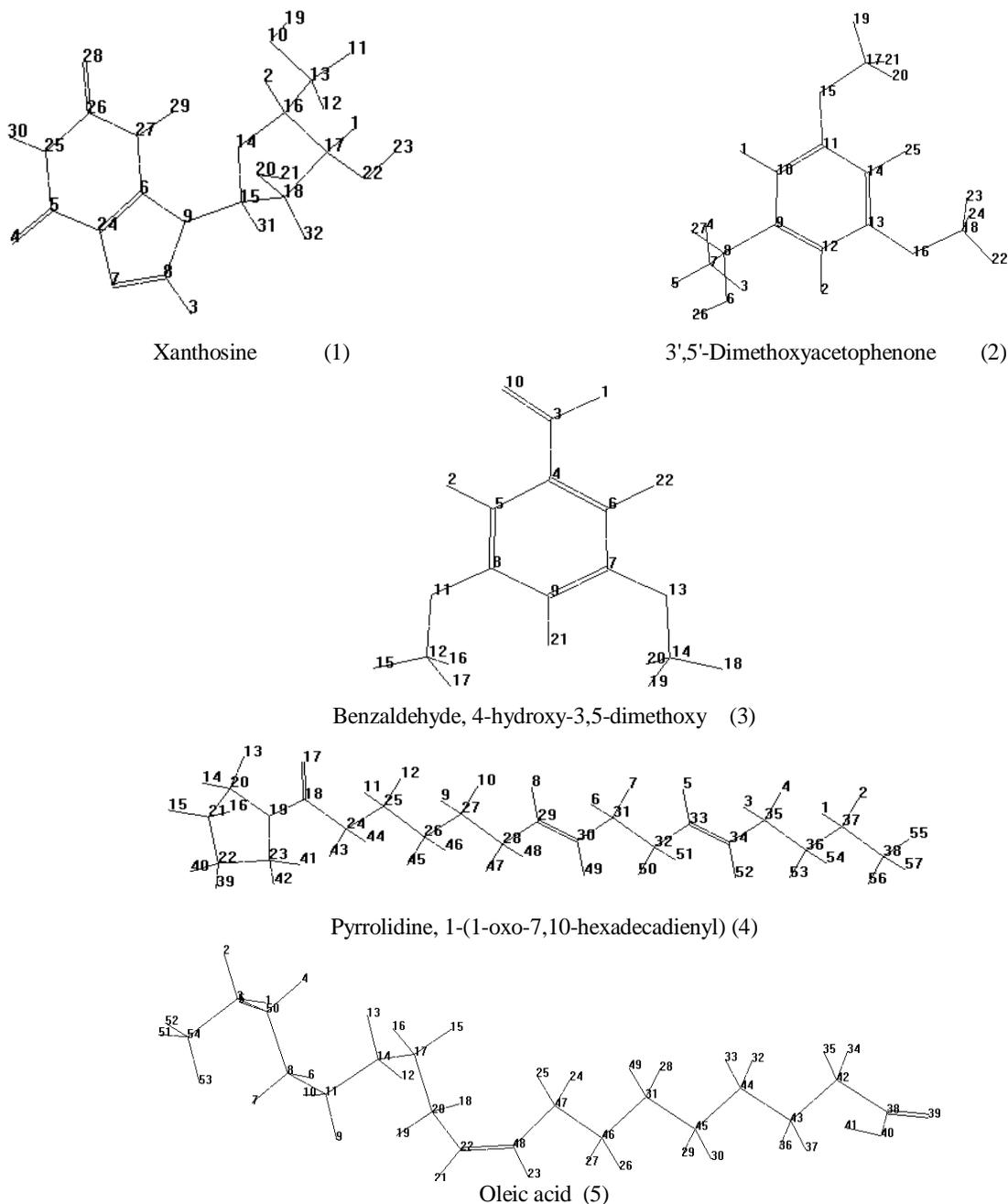
Xanthosine   (1)

3',5'-Dimethoxyacetophenone   (2)

Benzaldehyde, 4-hydroxy-3,5-dimethoxy   (3)

Pyrrolidine, 1-(1-oxo-7,10-hexadecadienyl) (4)

Oleic acid (5)

Fig. 5. The inhibitor molecules structure of the rape-cake extract obtained after a geometric optimization procedure using HyperChem 7.0 computer package (RHF calculation, singlet state, PM3 parameterization)
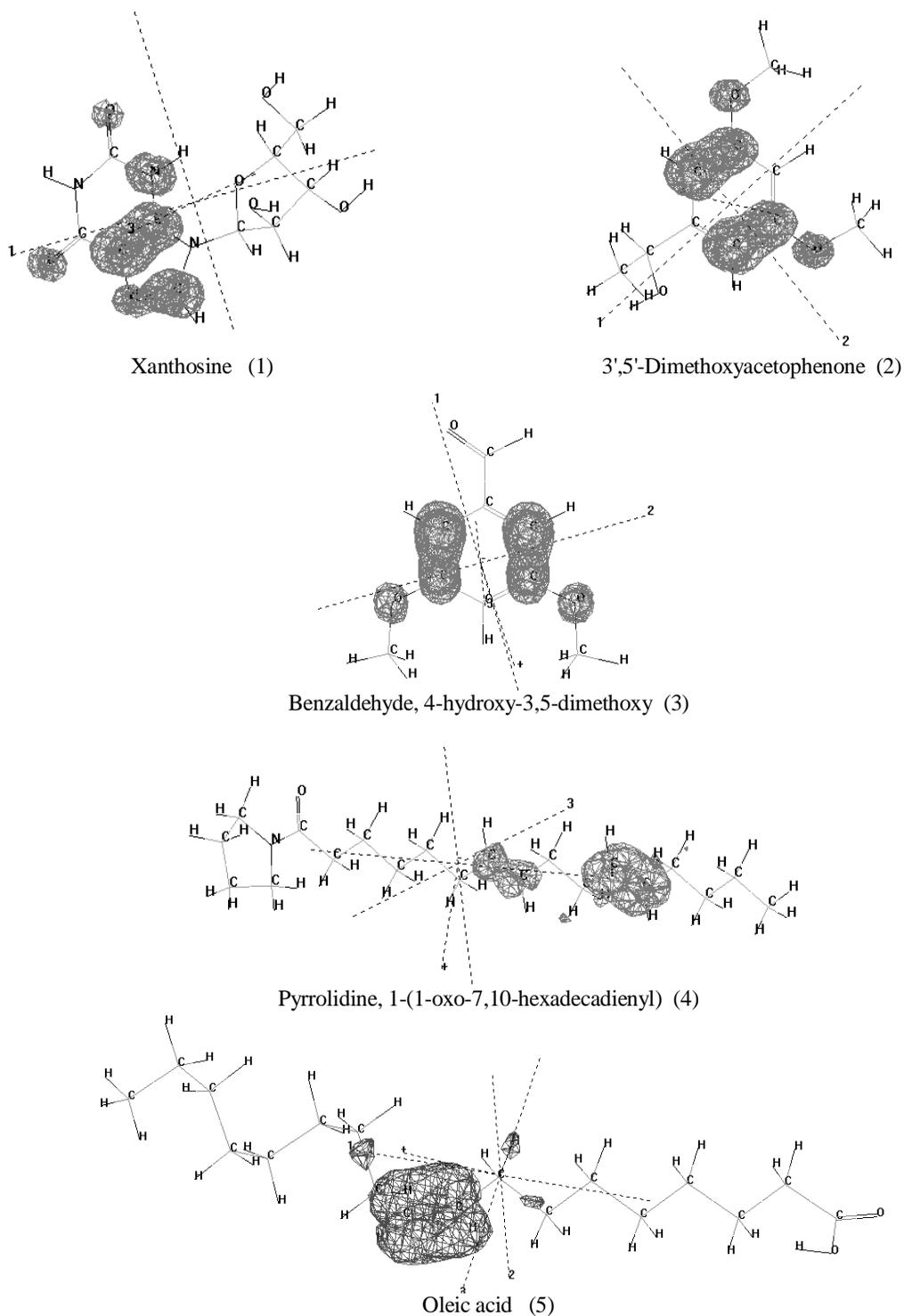
Xanthosine   (1)   3',5'-Dimethoxyacetophenone (2)

Benzaldehyde, 4-hydroxy-3,5-dimethoxy (3)

Pyrrolidine, 1-(1-oxo-7,10-hexadecadienyl) (4)

Oleic acid   (5)

Fig. 6. Optimized structures of inhibitor molecule 1-5. Density of the highest occupied molecular orbital is shown as a meshed isosurface (orbital density value is equal to 0.005)

Table 2

Quantum chemical parameters calculated by DFT

Molecule	E_{HOMO}, eV	E_{LUMO}, eV	ΔE_{L-H}, eV	Ionization potential
Xanthosine	-8.973	0.217	9.19	8.973
3',5'-Dimethoxyacetophenone	-9.081	0.211	9.29	9.081
Benzaldehyde, 4-hydroxy-3,5-dimethoxy	-9.440	-0.686	8.75	9.440
Pyrrolidine, 1-(1-oxo-7,10-hexadecadienyl)	-9.759	0.983	10.74	9.759
Oleic acid	-9.883	0.907	10.79	9.883

Table 3

Absolute hardness (χ), absolute electronegativity (η), softness (σ) and the number of electrons transferred between the inhibitor molecules and iron (ΔN) for the investigated compounds

Molecule	χ, eV	η, eV	σ, eV	ΔN
Xanthosine	4.37	4.60	0.21	0.285
3',5'-Dimethoxyacetophenone	4.43	4.64	0.21	0.276
Benzaldehyde, 4-hydroxy-3,5-dimethoxy	5.06	4.37	0.22	0.221
Pyrrolidine, 1-(1-oxo-7,10-hexadecadienyl)	4.38	5.37	0.18	0.243
Oleic acid	4.48	10.79	0.18	0.232

It can be seen that the most favourable sites for the interaction with the metal surface were the following atoms:

O10, O11, O13 with charges -0.294, -0.273, -0.276 for benzaldehyde, 4-hydroxy-3,5-dimethoxy;

O6, O15, O16 with charges -0.315, -0.278, -0.276 for 3',5'-dimethoxyacetophenone;

N25, N27, N7, N9, O4, O10, O14, O20, O22, O28 with charges -0.394, -0.305, -0.089, -0.195, -0.331, -0.307, -0.296, -0.309, -0.307, -0.368 for xanthosine;

O17, N19 with charges -0.358, -0.452 for pyrrolidine, 1-(1-oxo-7, 10-hexadecadienyl);

O39, O40 with charges -0.300, -0.271 for oleic acid.

When the HOMO orbital for these molecules is analysed (Fig. 6) it is found that the highest occupied molecule orbital (HOMO) is in the O11, O13 and C5, C8, C6, C7 for benzaldehyde, 4-hydroxy-3,5-dimethoxy, being the preferred zone for nucleophilic attack.

For xanthosine the HOMO is localized over the nitrogen atoms N27 and N7, and oxygen atom O28 and O24, being the favourite sites for interaction with the metal surface.

One can see that in 3',5'-dimethoxyacetophenone molecule (Fig. 6(2)) O6, O15, O16 carry more negative charges while C10, C11, C12, C13 carry more positive charges. This means that O6, O15, O16 are the negative charge centres, which can offer electrons to the Fe atoms to form coordinate bond and C10, C11, C12, C13 are the positive charge centres, which can accept electrons from orbital of Fe atoms to form feedback bond.

For oleic acid the HOMO is localized only over C22 and C48 the carbon atoms (–C=C–), being the favourite sites for interaction with the metal surface. It is found that the highest occupied molecule orbital (HOMO) is in the C29, C30, C33 and C34 for pyrrolidine, 1-(1-oxo-7.10-hexadecadienyl), being the preferred zone for interaction with the metal surface. In order to obtain more information about the electronic interaction of the inhibitor molecules with the metal surface the frontier orbital energy such as E_{HOMO}, E_{LUMO}, energy difference (ΔE), are used to rationalize the reactivity of the inhibitor molecule and molecule orbital coefficient (Table 2).

The HOMO energy (E_{HOMO}) is often associated with the electron donating ability of the molecule, whereas the E_{LUMO} indicates the ability of the molecule to accept electron. Therefore, high values of the E_{HOMO} indicate an increased tendency of the inhibitor to donate electron to the vacant d-orbital of Fe in mild steel. According to Wang et al. [31], high values of the E_{HOMO} facilitate adsorption and enhance inhibition efficiency by influencing the transport process through the adsorbed layer. The highest E_{HOMO} values are obtained for xanthosine, 3',5'-dimethoxyacetophenone and benzaldehyde, 4-hydroxy-3,5-dimethoxy.

Large values of the energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$) implies increased electronic stability and low reactivity, while low values render good inhibiting efficiency because the energy to remove an electron from the last occupied orbital will be low [32]. The smaller HOMO–LUMO energy gap implies soft–soft interaction

will be expected. The inhibitor energy gap increases in the order benzaldehyde, 4-hydroxy-3,5-dimethoxy < xanthosine < 3',5'-dimethoxyacetophenone < pyrrolidine, 1-(1-oxo-7,10-hexadecadienyl) < oleic acid indicating that the latter stable molecule is the strongest inhibitor.

The values of χ, η, σ and ΔN for the molecules are shown in Table 3.

The values of the fraction of electrons transferred (ΔN) suggest that the inhibitor electron donor strength increases in the same order as the dipole moment [29, 30]. The value of ΔN shows inhibition effect resulting from electrons donation. It means if $\Delta N < 3.6$ (as obtained in this study) the inhibition efficiency increases with the increase of electron donating ability at the metal surface. In this study the inhibitor molecules of the rape-cake extract are the electron donors and the mild steel surface is the acceptor, thereby binding the inhibitor molecules to the mild steel results in inhibition adsorption layer against corrosion. The inhibition potential of 2-propanol of rape-cake extract is attributed to the presence of glycosides, ketone and aldehyde.

4. Conclusions

1. A novel volatile corrosion inhibitor (VCI), rape-cake extract, was developed for temporary protection of carbon steel; the maximum inhibition efficiency is about 93 %.

2. Rape-cake extract suppressed the anodic reaction of steel electrode and renders the corrosion potential to more noble direction.

3. The volatile chemical composition of rape-cake extract is highly complex containing glycosides, nucleosides, ketone, aldehyde, fatty acids, sterol, and alkaloids.

4. The inhibition action of the extract was attributed to the presence of aldehyde, ketone, and glycosides. The application of the main compounds calculations has been very successful and can be used to understand the inhibition process of corrosion.

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ДОСЛІДЖЕННЯ ЕКСТРАКТУ ШРОТУ РІПАКУ ЯК ЕКОЛОГІЧНО БЕЗПЕЧНОГО ЛЕТКОГО ІНГІБІТОРУ КОРОЗІЇ

Анотація. *Екстракт шроту ріпаку досліджений як новий леткий інгібітор атмосферної корозії сталі. Методом газової хромато-мас-спектрометрії отримано компонентний склад його летких фракцій. З використанням програми HyperChem7.00 були проведені квантово-хімічні розрахунки основних компонентів екстракту.*

Ключові слова: *екстракт шроту ріпаку, леткий інгібітор корозії, квантово-хімічні розрахунки.*