FROM CORROSION OF METALS FROM OIL SEPARATIVE ORGANIC COMPOUNDS USE IN PROTECTION

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ANNOTATION

The article studies the inhibiting properties of 3-butylbenzothiophene and 5-acetyl-2-methylthiaindanesulfoxide in a solution of hydrochloric and sulfuric acid. It was found that the studied compound exhibit very good inhibiting properties in acid corrosion.

Keywords: ***inhibitor, corrosion, sulfoxide, benzothiophene, thiaindane, electron-withdrawing group, electron-donor group, cell, orbital***.

Without metal equipment, all areas of the economy, including the chemical, oil, and gas industries, are difficult to comprehend today. When this equipment is employed in all areas of the economy, it is constantly in contact with the external environment, and the original properties of metal equipment are lost as a result of these interactions. As a result of contact with the external environment, oxides and hydroxides of the metals being exploited develop, resulting in the failure of metal-based equipment. Environmental contamination is caused by the iron oxides and iron hydroxides generated as a result of these activities.

One of the most common types of corrosion in the oil business is general and local corrosion. Internal corrosion [1; 2104-2113 p], which is mostly manifested in the formation of corrosion cracks under various stresses, is another key problem encountered in the functioning of pipes. The addition of corrosion and erosion is a key concern of pipe erosion, according to Martines and co-authors [2; 255-258 b]. Due to the combined usage of various materials, the incidence of galvanic corrosion has recently increased. Wilhelm [3; 691-703 p] demonstrates that the connection of corrosion-resistant steel pump-compressor pipes with a low-quality steel column is a common case of material accumulation in drilling wells. Furthermore, the bonding metals create cracked corrosion in the space between the pipe and the column. Hydrochloric acid is also used to keep salts from building up in metals used in oil extraction, drilling, gas purification, and industrial. Acidic corrosion of the metal surface results as a it of this.

Acidic corrosion of the metal surface results as a result of this. The development of inhibitory systems to protect metals from corrosion in various areas of the economy is of special practical and theoretical importance in nations with fast rising world industries.

Organic sulfur compounds in concentrated form are particularly effective at protecting metals from corrosion in acidic environments and can be used as the primary corrosion inhibitor in a variety of industries. It is required to apply bitumen production technologies in a suitably targeted manner in order to obtain these products in big quantities.

Their primary source of raw material is a residual percentage of high-sulfur oil. We have our own [4; in our article 4543-4548. p], we go through the inhibitory effects of thiaidan and thiochroman -aminocetones from this class against electrochemical corrosion in acidic conditions in great detail.

One of the most important and cost-effective techniques, we believe, is naturally isolating the bicyclic sulfur organic compounds contained in the heavy component of oil and increasing their use as effective inhibitors in the corrosion protection of metals. The inhibitory effect of 3-butylbenzo [b] thiophene (I) and 5-acetyl-2-methyltiaindensulfoxides (II) isolated from oil in the protection of metals from acid corrosion was studied in temperature ranges using gravimetric methods at 20 percent hydrochloric acid and 30 percent sulfuric acid 25 0S and 75 0S. The tests were carried out on a St.235 sample that was shaped into a dimensional plate with a height of 100 mm, a thickness of 20 mm, and a width of 20 mm. The study took 4 hours to complete. The tests were carried out in 250, 500, and 1000 mg/l solutions of inhibitory compounds. The corrosion protective effect of metals in a 20 percent hydrochloric acid solution of 3-butylbenzothiophene molecule was less significant in the additional solutions of 250 mg/l and 500 mg/l, according to the findings. The corrosion protection efficacy of metals was shown to be 55 percent at 25 0S and 75 percent at 75 0S in a solution of 1000 mg / l of this chemical. The corrosion protection efficacy of the 5-acetyl-2-methyltiaindensulfoxide molecule at 250 mg/l was determined to be 90.5 percent at 25 ° C and 76 percent at 75 ° C under the same conditions.When the efficiency of corrosion protection of metals was investigated, it was discovered that the amount of 500 mg / l of this material was 92.5 percent at 25 ° C and 81 percent at 75 ° C. When the effectiveness of corrosion protection of metals in a 1000 mg/l solution of the same substance was investigated, it was discovered to be 94 percent at 25 0S and 85 percent at 75 0S. Tables 4.1 and 4.2 show the results of the gravimetric method on the degree of corrosion protection of metals of the above-mentioned compounds.

3-butylbenzothiophene and 5-acetyl-2-methylbenzothiophene St.235 steel for 4 hours at 25 0S and 75 0S the effectiveness of protecting the sample in 20% HCl solution

Table 4.1

combination number	Concentration, mg / l	Temperature 25 ^{0}C		Temperature 75 ^{0}C	
		Corrosion speed, $K_{г/м^2 \cdot с}$	Protection level, (Z), %	$K_{г/м^2 \cdot с}$	Protection degree, (Z), %
I	250	-	-	-	-
	500	-	-	-	-
	1000	9,0	55	388	75
II	250	2,1	90,5	359	76
	500	1,5	92,5	289	81
	1000	1,3	94	197	85

The degree of corrosion protection of metals of both substances reduces with rising temperature in a hydrochloric acid environment, as shown by the preceding data. This means that in any chemical process, an increase in temperature generates an increase in the reaction rate, according to the Le Chatelee principle. The direct presence of an oxygen atom in the carbonyl group and a sulfur-bonded molecule in this molecule explains why its acetylsulfoxide exhibits inhibitory effects even at low concentrations as compared to alkylbenzothiophene.

An increase in the concentration of impurities used as inhibitors from 250 mg/l to 1000 mg/l directly demonstrated that these compounds led to an increase in the inhibitory characteristics' efficiency in metal corrosion prevention. When the corrosion protection efficacy of metal II utilized as an inhibitor was compared, it was discovered that its inhibitory qualities were stronger at 25 0S (94%) than at 75 0S. (85 percent).

Under the above conditions, the efficiency of corrosion protection of metals of the same compounds in a 30 percent sulfuric acid medium was investigated using a gravimetric method. The results of the study are presented in Table 4.2 below. From the data in the table, it can be concluded that the corrosion protection efficiency of substances I of metals was not significantly affected at 250 and 500 mg / l, as in the above hydrochloric acid environment. However, the inhibitory properties of a 1000 mg / l solution of this substance I were found to be 62% at 25 ° C and 59% at 75 ° C.This suggests a minor rise in inhibitory property in a sulfuric acid environment at a temperature of 25 0C, and a decrease in inhibitory property at a temperature of 75 0C. Based on the findings of the investigation of substance II's inhibitory qualities on the efficacy of corrosion protection of metals, it can be concluded that as the temperature and concentration of the substance increased, so did the inhibitory effect of this compound.

3-butylbenzothiophene and 5-acetyl-2-methylbenzothiophene St.235 steel for 4 hours at 25 0S and 75 0S the effectiveness of protecting the sample in 30% H_2SO_4 solution

Table 4.2

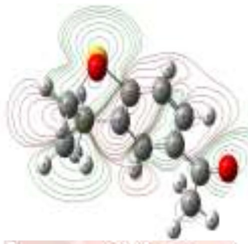
Combination number	Concentration, mg / l	Temperature 25 ^{0}C		Temperature 75 ^{0}C	
		Corrosion speed, $K_{г/м^2 \cdot с}$	Protection level, (Z), %	$K_{г/м^2 \cdot с}$	Protection degree, (Z), %
I	250	-	-	-	-
	500	-	-	-	-
	1000	12,5	62	577	59
II	250	2,1	93	33	97,5
	500	1,5	94,7	3,9	99,7
	1000	1,3	96,0	1,8	99,8

Quantum chemical approaches are still one of the most affordable, practical, and universal ways for examining the electronic structure of molecules today. In any reaction, a molecule's activity is mostly determined by its structure and energy characteristics. Chemists were able to plan experimental work and undertake targeted product synthesis thanks to the advent of quantum chemical methods of calculation. Many contemporary computing systems now give quantum chemistry and molecular dynamics data all around the world. The HyperChem program, on the other hand, is one of the most commonly accepted ways for getting quantum chemical computations and molecular dynamics data. The electronic structure and quantum chemical computations of 5-acetyl-2-methyltiaindensulfoxide were investigated using HyperChem 7.0, Semi-empirical method-PM3, (AM1), Algorithm-Polak-Riebiere versions [1151; 28-32 pp] based on the aforesaid approaches.

The data collected using the RMZ and AM1 semi-empirical methods from the 5-acetyl-2-methyltiaindensulfoxide molecule are shown in the following figures.

3D structure of sulfoxide formula

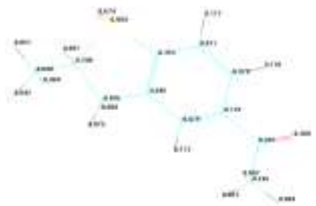
Distribution of atomic charges in a sulfoxide molecule



HOMO molecular orbital of sulfoxide

LUMO molecular orbital of sulfoxide

The total charge density of sulfoxide



Bond energy of sulfoxide

It's worth noting that, in addition to the upper complete binding (HOMO) molecular orbitals, the lower unoccupied (free, free) relaxing molecular (LUMO) orbitals play a significant role in understanding the energies of atomic orbitals. The energy of HOMO-orbitals describes the electron donor properties of molecules, whereas the energy of LUMO-orbitals describes the molecule's ionization potentials. The energy of LUMO-orbitals in the molecule has electron-accepting characteristics. As a result, the higher the energy of HOMO-orbitals in organic molecules, the easier it is for electrons to transfer electrons to a molecule's atom with another electron deficiency.

Quantum chemical calculations of the same chemicals are also useful in elucidating the mechanism of the 5-acetyl-2-methylthian indansulfoxide molecule examined in this study in the process of metal inhibition. As a result, in the inhibitory mechanism of organic molecules utilized in corrosion processes, the higher the energy of electrons in the binding orbitals, the easier it is to transfer electrons to the vacant orbital cells in the d-step of iron. This means that the high energy in the binding energy orbitals of the inhibitors utilized shows that this chemical has a high anticorrosive action.

The oxygen and sulfur atoms have the most negative charge in the molecule, according to an analysis of the molecule's effective charge quantities. The electron density in the molecule is fairly dense around these atoms, as can be shown. Due to the density of electrons in the donor-acceptor bonds, the applied molecule wave function and neplanar configuration of the molecule suggest that this molecule covers positively charged particles on the metal surface while protecting the metal from corrosion. This process is aided by parts of the molecule with the high electron density discussed earlier. The process of physical adsorption, which protects the inhibitors in this form, can be used to explain the corrosion of metals. It also resists corrosion on the metal surface by focusing its electrons on the unfinished d-stage of iron at the expense of the molecule's other atoms. Chemical adsorption can be used to explain this phenomenon. In conclusion, sulfur-containing organic molecules produced from petroleum can be used as effective inhibitors that are also environmentally beneficial.

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