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**INHIBITION OF CORROSION WITH ORGANIC COMPOUNDS IN THE WATER AND SALT AND ACID MEDIUM. THE ASPECT OF ISOMERISM AND THE INTERCLASS ASPECT OF THE INHIBITION PROCESS**

**ИНГИБИРОВАНИЕ КОРРОЗИИ ОРГАНИЧЕСКИМИ СОЕДИНЕНИЯМИ В ВОДНОЙ СРЕДЕ С АГРЕССИВНЫМ КОМПОНЕНТОМ. АСПЕКТ ИЗОМЕРИИ И МЕЖКЛАССОВЫЙ АСПЕКТ ПРОЦЕССА ИНГИБИРОВАНИЯ**

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*Abstract.* In this paper, the process of adsorption of phenol derivatives, polyaminopolycarboxylic acids (PFPA) and tertiary amine salt, modeled on semi-empirical ZINDO/1, on iron (available in different grades of steel in the amount of 90-97%) is presented. The structures of the phenol derivatives for the study were chosen without complicating the structure, and the isomers of the position of the substituents were chosen. The structures of polyaminopolycarboxylic acids for the study were chosen according to the structure complication. In the course of the study, the following compositions were obtained and analyzed: compositions of the complexes obtained, global and local electrophilicity values, a graph showing the dependence of the charge density on the iron atom on the protective effect. For the first time, the interclass aspect of corrosion protection will be considered, where the generality of the investigated quantum-chemical approach for different classes of organic inhibitors, which are also found in different corrosive environments, will be proved.

*Аннотация.* В публикуемой работе представлен смоделированный посредством полуэмпирического ZINDO/1 процесс адсорбции производных фенолов, полиаминополикарбоновых кислот (ПФПК) и соли третичного амина, на железе (имеющегося в разных сортах стали в количестве 90-97%). Структуры производных фенолов для исследования были выбраны без усложнения структуры, а были выбраны изомеры положения заместителей. Структуры полиаминополикарбоновых кислот для исследования были выбраны согласно усложнению структуры. В процессе исследования были получены и проанализированы: составы полученных комплексов, глобальных и локальных величин электрофильности, график, отображающий зависимость плотности заряда на атоме железа от защитного эффекта. Впервые будет рассмотрен межклассовый аспект защиты от коррозии, где будет доказана общность исследуемого квантовохимического подхода для разных классов органических ингибиторов, находящихся также и в разных коррозионных средах.

*Keywords:* polyaminopolycarboxylic acids, phenol derivatives, tertiary amines, sodium chloride, n-octane, steel corrosion, chemical adsorption, partial effective charges

*Ключевые слова:* полиаминополикарбоновые кислоты, производные фенолов, третичные амины, хлорид натрия, n-октан, коррозия стали, химическая адсорбция, парциальные эффективные заряды

*List of author's abbreviations*<sup>1</sup>:

OC - organic compound

R is a *n*-amyl radical

Z% - protective anticorrosive effect: inversely proportional to the rate of corrosion

$\omega_{gl}$  is global electrophilicity of the OC molecule

$Q_S$  is the charge on the sulfur atom

$Q_O$  is charge on the oxygen atom of phenolic hydroxyl

$Q_{CH_3}$  is a charge on a methyl group forming a group of atoms

$Q_{RCH_3}$  is a charge of the methyl group on the radical *n*-amyl

$Q_{p-CH_3}$  is the charge of the methyl group in the *para*-position of the benzene ring with respect to the phenolic hydroxide

$Q_{o-CH_3}$  is the charge of the methyl group in the *ortho*-position of the benzene ring with respect to the phenolic hydroxide

$\Sigma_B Q_C$  is the total charge of carbon atoms of the benzene ring

$Q_N^+$  is the charge on the nitrogen atom of the  $-NH_3^+$

$Q_N$  is the charge on the nitrogen atom of the cysteine fragment of glutathione

${}_{p.b.} Q_O$  is the charge on the oxygen of the keto group near the cysteine fragment

${}_k Q_O$  is the charge on the oxygen atom of the keto group of the cysteine fragment

${}_h Q_O$  is the oxygen atom of hydroxyl of cysteine

${}_{k \text{ near } N^+} Q_O$  refers to glutathione: an oxygen atom of the keto group located near the nitrogen atom of the  $-NH_3^+$

${}_{h \text{ near } N^+} Q_O$  refers to glutathione: an oxygen atom of the hydroxy group located near the nitrogen atom of the  $-NH_3^+$

${}_{k \text{ near } N} Q_O$  refers to glutathione: an oxygen atom of a keto group located near the nitrogen atom of the  $-NH-$

${}_{h \text{ near } N} Q_O$  refers to glutathione: an oxygen atom of the hydroxy group located near the nitrogen atom of the  $-NH-$

$\Sigma Q_{C=C}$  is the total charge on carbon atoms in the double bond contained in the tertiary amine salt molecule

${}_{-CN} Q_N$  is the charge on the nitrogen atom of the nitrile group contained in the tertiary amine salt molecule

Corrosive aggressiveness of phenols is usually very low, and some of them are good corrosion inhibitors. Phenols are highly soluble in fuel, do not form precipitation during oxidation, do not cause corrosion of structural materials, etc. That is why, the effectiveness, antioxidant additives based on alkylphenols are widely used [14]. They were also applied to microbiological corrosion [22], their effectiveness was estimated by comparing the structure-property correlation coefficients.

A lot of work has been done with water-soluble inhibitors, which are a product of the condensation of various phenols (coal, slate) with ethylene oxide. As a result of the research and

<sup>1</sup> The remaining abbreviations found in the text are generally accepted

testing of various surface active substances of this class, it was found that phenols condensed with 8-10 moles of ethylene oxide were effective as oil inhibitors under oil-water conditions when pumped into a well at the rate of 200 g / ton of produced water, that, applying it, you can brake hundreds of times the underground corrosion of steel. Under these stringent test conditions, oxyethylated phenols proved ineffective in protecting both ferrous and non-ferrous metals.

The high anticorrosive activity and perspectivity of the use as active components of corrosion inhibitors of hydroxyethylaminomethyl and sodium sulfonatomethyl derivatives of *para*-isononylphenol, as well as oligomeric products of its condensation with formaldehyde [15] have been established. The synergetic character of the anticorrosive effect of the joint use in the corrosion inhibitors of the hydroxyethylaminomethyl and sodium sulfonatomethyl derivatives of *para*-isononyl phenol [16] has been revealed.

The role of the centers of adsorption of molecules of phenol derivatives on the surface of corrosive iron is performed by aromatic systems that are oriented parallel to the surface of iron due to the interaction of electrons of all double bonds with atoms of its surface, and we are also allowed dissociative adsorption, which creates the possibility of the formation of surface  $\pi$ -complexes [23]. Data were obtained on the anticorrosion activity of substances named by the authors [20] “phenol sulfides”, then this name will be used in this article, because they are the basis of the narrative. Further, they will be suggested that an inhibitor of the “two in one” type.

Since the main idea is a test of phenolsulfides, I will only briefly mention polyaminopolycarboxylic acids. Related compounds - polyaminopolycarboxylic acids have been investigated in the work (calculation of correlation coefficients “protective effect of corrosion - quantum chemical descriptor”) [17, 36], the chemisorption interaction of 2-aminopropanoic acid adsorption centers was also modeled (one of the author's first works in this direction) on 4 iron atoms [21]. And a similar study of complexones, in particular, NTA and EDTA [11] and some others. Now positive charges on the nitrogen atom help to show high, but not so high, protective effects as phenolsulfides.

Amines (including protonated, and therefore having a center of physical adsorption [13]) have long been common, and have been studied in a large number of works [18, 19].

### *Methods*

#### *A variety of corrosion system*

6 representatives act as inhibitors of corrosion, added at a concentrations 50 mg / L and 200 mg / L contained in a closed system (this is a tube with a volume of 0.400 L).

Samples of steel were parameters 20×50×1 mm. Samples of steel were taken from one batch, which guaranteed them the same chemical composition [4].

#### *Phenolsulfides*

In [20], there is a corrosive closed thermodynamic system, “steel St3 / 3% NaCl”, for comparison Z%, a corrosive closed thermodynamic system of “3% NaCl + n-octane (7:1)” is mentioned.

#### *Polyaminopolycarboxylic acids*

In [24] there is a corrosive closed thermodynamic system “steel 20Г / 0.1M HCl”

#### *Tertiary amine salt*

In [18] there is a corrosive closed thermodynamic system “steel St3 / 3% NaCl + 0.8 g / L H<sub>2</sub>S” (acidified with HAc, pH = 5)

*Using organic inhibitors and their method of application in the corrosion system*

*Phenolsulfides*

3 representatives were selected. The decoding of the code symbols of Figure 1 is given in Table 1 (Fig 1 and Table 1).

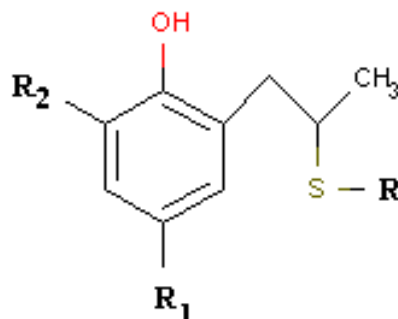


Figure 1. The general structure of the phenolsulfide molecules

Table 1.

DECODING OF THE COMPOSITION OF THE RADICALS OF EACH MOLECULE OF PHENOLSULFIDES, ACCEPTED ABBREVIATIONS, GENERATED NAMES

The radical code	<i>pph</i> 2-[2-(pentylsulfanyl)propyl]phenol <sup>1</sup>	<i>4mpph</i> 4-methyl-2-[2-(pentylsulfanyl)propyl]phenol	<i>2mpph</i> 2-methyl-6-[2-(pentylsulfanyl)propyl]phenol
R	-pentyl	-pentyl	-pentyl
R <sub>1</sub>	-H	-methyl	-H
R <sub>2</sub>	-H	-H	-methyl

*Polyaminopolycarboxylic acids*

Two representatives were examined: cysteine or **cys**<sup>+</sup> (1-carboxy-2-sulfanylethan-1-aminium) and glutathione or **gln**<sup>+</sup> 1-carboxy-3-[[1-(carboxyamino)-1-oxo-3-sulfanylpropan-2-yl]carbonyl]propan-1-aminium, hereinafter referred to as the protonated forms of polyaminopolycarboxylic acids (or PFPA).

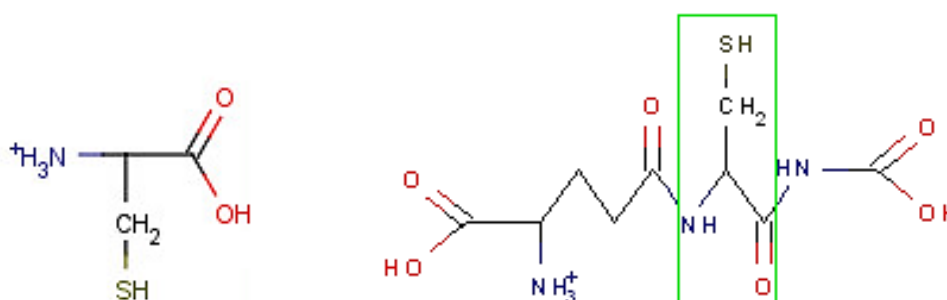


Figure 2. The general structure of PFPA

<sup>1</sup> The names and patterns of the molecules were generated with MarvinSketch program 5.2.4

The author conventionally accepted that just such a protonation corresponds to the presence of these corrosive media.

*Tertiary amine salt*

One representative was investigated, viz. butyl(2-cyanoethyl)(3-ethoxy-3-oxoprop-1-en-1-yl)azanium chloride or **bac**<sup>+</sup>

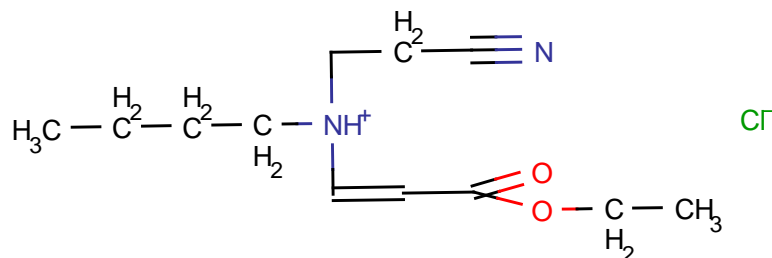


Figure 3. The general structure of the molecule of the tertiary amine salt

*The protective effect against corrosion*

The Z% was published (in different concentrations) in<sup>1</sup> [18, 20, 24], therefore the inhibitory effect of these compounds has been proven. According to [18, 24], the above structure was a structural series of molecules.

*The technology of quantum chemical calculations*

The quantum chemical experiment was carried out with HyperChem 8.0.7, using the built-in visualization tools according to the methodology expressed in [11, 12].

Peculiarities of this work is that phenolsulfides are colloidal surfactants, respectively, adsorption modeling is performed only taking into account the hydrophilic part (which can be adsorbed), since the long nonpolar R by [15, 22], impairs the adhesion of the molecule to the surface of the steel plate. Simulation of adsorption of other classes of OC occurs with an accuracy according to the standard procedure in [11, 12].

*Results and discussion*

*Charges to heteroatoms, electrophilicity values*

The generated quantum-chemical descriptors OC and  $Fe_a \leftarrow [OC Y]$  are presented in Tables 2 and 3:

The charge distribution shown in Table 2 indicates a very high charge difference  $\Sigma_B Q_C$  (recharging occurs),  $Q_S, -CN Q_N$  (recharging occurs).

**2mpph** shows a greater Z%, which is associated with 1) the activation of the benzene ring by a 1-type substitute 2) the absence of steric hindrance in position 3, 4, 5 of the benzene ring. High Z% in **2mpph** is also associated with low global electrophilicity in the iron complex.

The ZINDO/1 method shows a 10-fold increase in the global electrophilicity of phenolsulfides by the introduction of a methyl radical into the benzene ring, a 2-fold decrease in the global electrophilicity of PFPA when the cysteine is surrounded, and the molecule of the tertiary amine salt is not clear, because it is the only one.

In molecules of iron complexes of phenolsulfides, the global electrophilicity is greater than in the initial ones, in the molecules of PFPA iron complexes, the global electrophilicity is also greater than in the initial ones. This indicates a strong degree of transition of the electron density to iron. In the molecule of the iron complex of the tertiary amine salt, the global electrophilicity is also greater than that of the tertiary amine salt.

<sup>1</sup> Calculated by gravimetric method, mentioned in many works, including [1-10]

Table 2.

THE VALUES OF THE CALCULATED PARTIAL EFFECTIVE CHARGES  
 OF OC AND OF Fe<sub>a</sub> ← [OC Y]

Molecule code Y	Descriptor name	The value of the descriptor of the iron complex	The value of the descriptor of the initial OC	$\omega_{gl}$ of the initial OC	$\omega_{gl}$ of the iron complex
Pph	Q <sub>S</sub>	0.042	-0.318	$8.4 \times 10^{-4}$	1.20
	Q <sub>O</sub>	-0.159	-0.347		
	Q <sub>CH3</sub>	-0.122	-0.164		
	Q <sub>RCH3</sub>	-0.062	-0.137		
	$\sum_B Q_C$	0.972	-0.202		
4mpph	Q <sub>S</sub>	0.232	-0.315	$7.8 \times 10^{-3}$	1.23
	Q <sub>O</sub>	-0.116	-0.345		
	Q <sub>CH3</sub>	-0.129	-0.165		
	Q <sub>RCH3</sub>	-0.099	-0.137		
	Q <sub>p-CH3</sub>	-0.061	-0.153		
	$\sum_B Q_C$	1.102	-0.271		
2mpph	Q <sub>S</sub>	0.000	-0.316	$2.2 \times 10^{-3}$	0.97
	Q <sub>O</sub>	-0.125	-0.370		
	Q <sub>CH3</sub>	-0.087	-0.162		
	Q <sub>RCH3</sub>	-0.086	-0.137		
	Q <sub>o-CH3</sub>	-0.026	-0.142		
	$\sum_B Q_C$	1.072	-0.158		
Cys <sup>+</sup>	Q <sub>S</sub>	0.212	-0.235	1.24	8.22
	Q <sub>N<sup>+</sup></sub>	-0.044	-0.219		
	<sup>k</sup> Q <sub>O</sub>	-0.004	-0.477		
	<sup>h</sup> Q <sub>O</sub>	-0.127	-0.401		
Gln <sup>+</sup>	<sup>1</sup> Q <sub>S</sub>	0.178	-0.625	0.65	5.82
	Q <sub>N</sub>	-0.107	-0.211		
	<sup>k</sup> Q <sub>O</sub>	-0.065	-0.359		
	Q <sub>N<sup>+</sup></sub>	-0.049	-0.223		
	<sup>p.b.</sup> Q <sub>O</sub>	-0.133	-0.356		
	<sup>k</sup> near N <sup>+</sup> Q <sub>O</sub>	-0.026	-0.421		
	<sup>h</sup> near N <sup>+</sup> Q <sub>O</sub>	-0.140	-0.386		
	<sup>k</sup> near N <sup>+</sup> Q <sub>O</sub>	-0.120	-0.428		
<sup>h</sup> near N <sup>+</sup> Q <sub>O</sub>	-0.144	-0.325			
Bac <sup>+</sup>	Q <sub>N<sup>+</sup></sub>	-0.045	-0.045	1.24	5.55
	<sup>h</sup> Q <sub>O</sub>	-0.075	-0.329		
	<sup>k</sup> Q <sub>O</sub>	-0.139	-0.401		
	Q <sub>butCH3</sub>	-0.026	-0.143		
	Q <sub>ethCH3</sub>	-0.058	-0.177		
	-CNQ <sub>N</sub>	0.183	-0.314		
	$\Sigma Q_{C=C}$	0.474	0.015		

<sup>1</sup> The following 3 lines mean heteroatoms belonging to the cysteine fragment (this is a green frame)

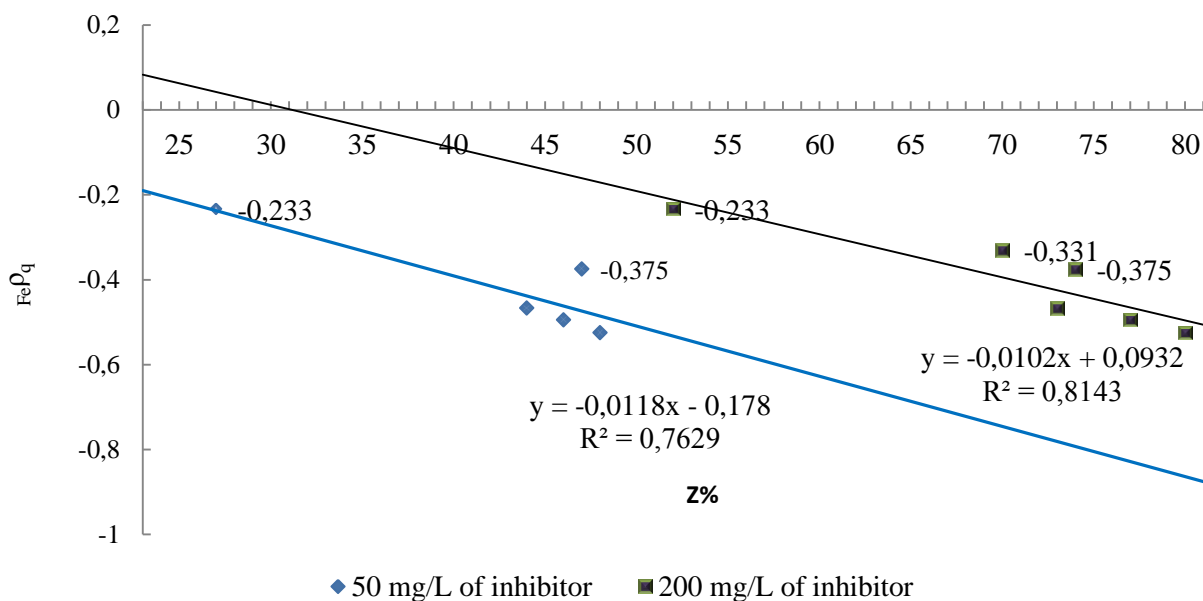
Table 3.  
 THE VALUES OF THE CALCULATED ENERGIES OF THE BOUNDARY ORBITALS  
 OF THE MOLECULES OF OC AND OF  $Fe_a \leftarrow [OC Y]$

Molecule code Y	pph	4mpph	2mpph	Cys <sup>+</sup>	Gln <sup>+</sup>	bac <sup>+</sup>
E (HOMO)	-7.551	-6.962	-7.236	-12.497	-9.054	-10.629
E (LUMO)	7.874	7.928	7.810	1.120	1.605	0.248
The composition of the iron complex	$Fe_{11} \leftarrow pph$	$Fe_{12} \leftarrow 4mpph$	$Fe_{10} \leftarrow 2mpph$	$Fe_{10} \leftarrow Cys^+$	$Fe_{18} \leftarrow Gln^+$	$Fe_{14} \leftarrow bac^+$
E (HOMO)	-7.370	-7.304	-7.058	-10.444	-10.789	-10.306
E (LUMO)	-0.623	-0.743	-0.226	-6.221	-5.257	-5.025

There is also a direct dependence of “Z%-E (HOMO) in the iron complex” which can be explained by a drop in the ionization energy. The magnitude of global electrophilicity in phenol sulfides is very small (at least in the interpretation of ZINDO/1), and in all classes of OCs it rises sharply with complexation, which indicates the high completeness of the transition of the electron density to iron atoms from heteroatoms — this causes Z% to reach 80%.

*The charge density and its graphical dependence on the protective effect*

The dependence of  $Fe\rho_q$  of the investigated OCs on the protective anticorrosive effect manifested by the OC in concentrations of 50 mg / L and 200 mg / L is shown in Figure 4:



Conditional signs:  $\blacklozenge$  and  $\blacksquare$ , with data signatures — Cys<sup>+</sup> ( $Fe\rho_q = -0.233$ ), Gln<sup>+</sup> ( $Fe\rho_q = -0.331$ ), BAC<sup>+</sup> ( $Fe\rho_q = -0.375$ ) entered in the heterogeneous system. For Gln<sup>+</sup>, the protective effect at a concentration of 50 mg is unknown

Figure 4. Dependence of the protective anticorrosive effect of the OS of different classes on the charge density on iron



On the presented graph, the dependence is the same as in similar works [11, 12]. It is obvious that the points corresponding to PFPA of cysteine and glutathione with high reliability fall on the straight lines formed by the points corresponding to phenolsulfides. In this paper, another aspect is revealed: the stability of adsorption complexes begins to play an important role (although the author cannot quantitatively calculate this stability, since no simulation method has yet been developed that allows taking into account the influence of the corrosive medium). There is no doubt that the corrosive medium is either a catalyst or a chemisorption inhibitor, therefore: 1) with the addition of *n*-octane [20], the complex is somehow destroyed, since non-polar fragments of hydrocarbons enter the nonpolar medium, the protective effect decreases, 2) the effect of  $\text{Cl}^-$  less and less on the iron complexes of phenolsulfides, 3) the influence of  $\text{H}^+$  is increasingly on the iron complexes of PFPA 4) the effect of  $\text{S}^{2-}$  is large on the iron-tertiary amine complexes, based on the global electrophilicity of the iron complexes.

*Characterization of S-Fe bonds.*

Representatives of these classes of organic compounds have a sulfur atom of the type C-S. Therefore, I will compare the S-Fe bonds with the upper threshold of 2.5 Å, as indicated above. The sulfur valence in the OC is not difficult to calculate from the data in Tables 4-8.

Atoms of sulfur are part of the phenol sulfide molecules in the form of  $\begin{array}{c} | \\ \text{---} \text{S} \text{---} \text{R} \\ | \end{array}$ , within **cys**<sup>+</sup> and **gln**<sup>+</sup>, the sulfur atom is present in the form of  $\begin{array}{c} | \\ \text{---} \text{S} \text{---} \text{H} \\ | \end{array}$ . In the PFPA of **cys**<sup>+</sup> and **gln**<sup>+</sup> there is no mesomeric effect over the entire area of the molecule. The data are presented in Tables 4-8:

Table 4.

CHARACTERIZATION OF S-Fe CHEMISORPTION BONDS INSIDE **Fe<sub>11</sub>←pph**

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.717	Fe-S	-1.31/-0.65	2.50
-0.563	Fe-S		

Table 5.

CHARACTERIZATION OF S-Fe CHEMISORPTION BONDS INSIDE **Fe<sub>12</sub>←4mpph**

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.556	Fe-S	-1,73 /-0,58	2.50
-0.460	Fe-S		
-0.714	Fe-S		

Table 6.

CHARACTERIZATION OF S-Fe CHEMISORPTION BONDS INSIDE **Fe<sub>10</sub>←2mpph**

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.607	Fe-S	-1.20 /-0.60	2.50
-0.605	Fe-S		



Table 7.

CHARACTERIZATION OF S-Fe CHEMISORPTION BONDS INSIDE  $\text{Fe}_{10} \leftarrow \text{Cys}^+$

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.251	Fe-S	-0.88 / -0.22	2.50
-0.100	Fe-S		
-0.194	Fe-S		
-0.330	Fe-S		

Table 8.

CHARACTERIZATION OF S-Fe CHEMISORPTION BONDS INSIDE  $\text{Fe}_{18} \leftarrow \text{Gln}^+$

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.482	Fe-S	-0.84 / -0.42	2.50
-0.354	Fe-S		

Atoms of iron are more strongly charged in phenolsulfides, from which a striking charge transfer is observed in phenolsulfides. PFPA has almost the same degree of charging, their poor protective properties are explained by the lack of mesomeric effect throughout the chain. High charge density gives high protective effects [11, 12].

*Characterization of N-Fe bonds.*

There is a relationship between PFPA and tertiary amine molecules in presence of nitrogen atoms of the amine type. The valence of nitrogen in the OC can be easily calculated from the data in Tables 9-11. The data are presented in Tables 9-11:

Table 9.

CHARACTERIZATION OF N-Fe CHEMISORPTION BONDS INSIDE  $\text{Fe}_{10} \leftarrow \text{Cys}^+$

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.251	Fe-NH <sub>3</sub> <sup>+</sup>	-0.80 / -0.27	2.50
-0.330	Fe-NH <sub>3</sub> <sup>+</sup>		
-0.218	Fe-NH <sub>3</sub> <sup>+</sup>		

Table 10.

CHARACTERIZATION OF CHEMISORPTION BONDS OF N-Fe INSIDE THE CYSTEINE FRAGMENT (THIS IS A GREEN FRAME) INSIDE  $\text{Fe}_{18} \leftarrow \text{Gln}^+$

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.376	Fe-NH-	-1.09 / -0.36	2.37
-0.237	Fe-NH-		2.50
-0.474	Fe-NH-		2.35

Table 11.

CHARACTERIZATION OF N-Fe CHEMISORPTION BONDS INSIDE  $\text{Fe}_{14} \leftarrow \text{bac}^+$

The charge of a specific iron atom	The name of bonds with heteroatoms	Total charge / average charge	The length of the quantum-chemically calculated bonds, Å
-0.360	$\text{Fe}-\text{NH}_3^+$	-0.85/-0.43	2.50
-0.493	$\text{Fe}-\text{NH}_3^+$		

Iron atoms are more strongly charged in  $\text{Fe}_{18} \leftarrow \text{Gln}^+$ , because the nitrogen atoms of the cysteine fragment are not ionized.

It is very likely that phenolsulfides have two inhibitors in one: I and II (Figure 5). This idea is based on the separation of the chemisorption centers by the hydrocarbon chain, possibly because the percentage of corrosion protection reaches 80%:

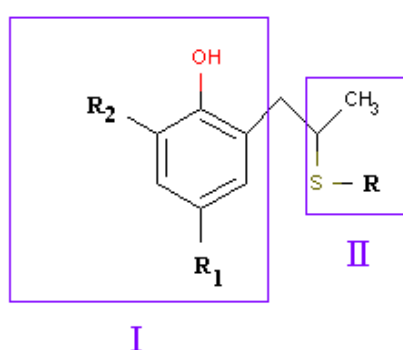
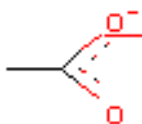


Figure 5. Possible distribution of the action of fragments

PFPA and tertiary amine salt have Z%, reaching up to 72%, because there is an anionic center



### Conclusion

Application of article approach, such as lack of hydration molecules, the use of pure iron atoms cluster instead of steel, semi-empirical methods of calculation and modelling obviously do not impose the print on the accuracy and predictive ability of the author improved cluster modeling theory. This enhancement allows you to get more information about protection of inhibitors of metal than the traditional and generally accepted theory. The improved method of quantum chemical modeling provides a much more comprehensive set of data that can serve as an effective tool for forecasting. Because iron complexes is not seen as superficial, and as an independent organic compound (or rather, the adduct) with well-defined chemical composition, is similar to  $\pi$ -complexes may be calculated as the actual value of the electronic tags last structure and function of Fukui. This represents a great promise, because currently the selection of microbial corrosion inhibitors increasingly performed quantum-chemical methods of prediction, not a screening method [1-7].

There is no doubt that a significant role in shaping improvements quantum chemical modeling belongs to the tremendous development of the power of new versions of quantum chemical programs, as well as the full development of visual imaging software. As soon as supercomputers are increasingly becoming an essential attribute of any area of the economy, all of the above approach will be less needed along with an increase in the level of quantum-chemical theory.

First of all, the author notes that the improved method yields reproducible results for all classes of organic compounds. The main adsorption centers can be easily traced from the change in the values of the programmed quantum-chemical descriptors: a stronger change will be observed if the descriptor is decisive in the manifestation of adsorption. These are sulfur atoms, benzene rings, double and triple bonds, nitrogen atoms.

#### Competing interests

The author declares that they have no competing interests.

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