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**QUANTUM-CHEMICAL SUBSTANTIATION OF CORROSION
INHIBITION OF STEEL WITH SOME AMINO ACIDS**

**КВАНТОВО-ХИМИЧЕСКОЕ ОБОСНОВАНИЕ ИНГИБИРОВАНИЯ
КОРРОЗИИ СТАЛИ НЕКОТОРЫМИ АМИНОКИСЛОТАМИ**

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Abstract. The article describes the process of α -amino acid adsorption on iron of mild steel immersed in 0.01 M H_2SO_4 , this process was modeled using HyperChem 8.0.8 and ZINDO/1. This method reflects the protection against corrosion by chemisorption of α -amino acid on the surface of metal to form a complex adduct, reliably. The compositions of obtained complexes, the energy of boundary orbitals, a graph depicting the dependence of the charge density on the iron atom and the energy of higher occupied molecular orbitals on the anticorrosive protective effect were obtained and analyzed. On the graphs one can see the equations of lines.

Аннотация. В статье описан процесс адсорбции органических соединений класса α -аминокислот на железе мягкой стали, погруженной в 0,01 М H_2SO_4 , Данный процесс был смоделирован используя HyperChem 8.0.8 и ZINDO/1. Такой метод отражает защиту от коррозии путем хемосорбции органического соединения на поверхности металла с образованием комплексного аддукта достоверно. В рамках исследования были получены и проанализированы: составы полученных комплексов, энергии граничных орбиталей, график, отображающий зависимость плотности заряда, приходящегося на атом железа, и энергии высшей занятой молекулярной орбитали от антикоррозионного защитного эффекта. На графиках можно видеть уравнения прямых.

Keywords: amino acids, protective anticorrosive effect, corrosion inhibitor, chemical adsorption, mild steel, the charge density per iron atom, partial effective charges, complex compounds, donor and acceptor bonds.

Ключевые слова: аминокислоты, защитный антикоррозионный эффект, ингибитор коррозии, химическая адсорбция, мягкая сталь, плотность заряда на атоме железа, парциальные эффективные заряды, комплексные соединения, донорно–акцепторные связи.

In this review, there are articles (Open Access), which feature molecules of amino acids (AA), protecting the steel of different brands from corrosion. Chronology is a middle of the 1990's to the present day. The articles are indexed in Scopus and Mendeley, special attention is paid to articles published by Elsevier.

It can be concluded that there is insufficient research by Russian authors precisely of amino acid molecules as inhibitors of corrosion in various media [1]. In [2] Russian scientists made a suggestion about the negative influence of the anionic center (which really is) on the inhibitory properties of the molecule.

Amino acids and their derivatives as inhibitors of corrosion in various media have been investigated thoroughly by a number of foreign authors whose works have been magnificently described in a remarkable review [3], to which the author of this article cannot add anything. The review concerns articles [5–36]. Studies in this field are still ongoing [4].

Methods

A variety of corrosion system

The corrosion occurred within 0.01 sulfuric acid.

The data (numbering of heteroatoms, the energy of the boundary orbitals of the initial molecules, the inhibition efficiency $Z\%$ at a concentration of 0.01 Mol / L, and 0.02 Mol / L) were taken from [5] for 9 α -amino acids (appearing in the scientific paper in the classical form (it is $\text{NH}_2\text{-CHR-COOH}$). Here is how it is described in [5]: «Skeleton I consisted of cysteine (CYS), serine (SER) and amino butyric acid (ABU). Those in skeleton II included threonine (THR), alanine (ALA) and valine (VAL) while those in skeleton III are aromatic amino acids, which included phenylalanine (PHE), tryptophan (TRP) and tyrosine (TYR)»

The technology of quantum chemical calculations

An improved method of quantum–chemical cluster modeling consisted: setting for program the maximum number of iron atoms (not surface ones, but isolated ones). The limiting number is x of it, when form of given–iron–atoms in the ground state ($x + b$) the b was carrying zero–charge (the x was charged by the charge $\Sigma\delta^-$).

Then it was postulated that AA's donor capabilities were exhausted.

The parallel plane of neutral iron–atoms specified by the HyperChem–user was 1.2 angstroms (A) away from the plane of AA so that the program produced fewer iterations and did not hang, which provides the necessary accuracy. The scaling of the calculations of the molecules studied in the program window (the Zoom–button) was 0.72.

The electrophilic reaction is $x\text{Fe}^0 + \text{AA} = \text{Fe}_x^{\Sigma\delta^-} \leftarrow \text{AA}^1$. The lengths of “Fe–adsorption center” bonds with a maximum 2.5 A length will be considered in some cases, bonds will be involved up to 2.7 A.

The determination of quantum chemical descriptors was carried out in 2 stages: 1) a) by optimizing the geometry with molecular mechanics method: first MM+, and then OPLS. b) setting the initial charge of AA with MNDO, 2) ZINDO/1. When specifying the original structure, local mesomeric effects inside AA were taken into account in the job–file.

The following descriptors of electronic structure were calculated: charges on heteroatoms of metalloids (by R. Mulliken) and charge density per iron atoms $\text{Fe}\rho_q$ (it is charge that accounts for 1

¹ Then the total degree of charge $\Sigma\delta^-$ will be ignored, I showed it then to explain what is the charge density per iron atom, i.e. $\Sigma\delta^- / x$

iron atom), the energy of boundary orbitals, and also the characteristics of bonds of resulting $Fe_x \leftarrow AA$ compounds. A set of Skeleton II differs from the others, since there is no significant range of Z%, and all amino acids of Skeleton II will donate identical fractions of electron density on iron atoms, therefore, the characteristics of bonds in chemisorption complexes for it will not be determined.

Results and discussion

The values

Partial effective charges on heteroatoms. The charge density per iron atom

The generated results of the quantum–chemical descriptors of electronic structure are summarized in tables 1–3.

Table 1.

THE VALUES OF THE CALCULATED QUANTUM CHEMICAL DESCRIPTORS OF AMINO ACIDS OF SKELETON I AND COMPLEX COMPOUNDS BASED ON IT

<i>Codes of corrosion inhibitors</i>	<i>CYS</i>	<i>SER</i>	<i>ABU</i>
Σq	-0.882	-1.269	-1.229
<i>Partial effective charges on heteroatoms*</i>	$5q_S = 0.050$	$5q_O = -0.328$	$7q_N = -0.271$
	$7q_O = -0.360$	$7q_O = -0.366$	$5q_O = -0.308$
	$6q_O = -0.304$	$6q_O = -0.308$	$6q_O = -0.362$
	$2q_N = -0.268$	$2q_N = -0.267$	$4q_N = -0.288$
<i>Empirical formulas of $Fe_x \leftarrow AA$</i>	<i>$Fe_{0.8} \leftarrow CYS$</i>	<i>$Fe_{0.9} \leftarrow SER$</i>	<i>$Fe_{0.9} \leftarrow ABU$</i>
Σq	-0.213	-0.477	-0.484
<i>Partial effective charges on heteroatoms</i>	$5q_S = 0.050$	$5q_O = -0.328$	$7q_N = -0.271$
	$7q_O = -0.360$	$7q_O = -0.366$	$5q_O = -0.308$
	$6q_O = -0.304$	$6q_O = -0.308$	$6q_O = -0.362$
	$2q_N = -0.268$	$2q_N = -0.267$	$4q_N = -0.288$
$F\sigma q$	-0.309	-0.254	-0.301

*An *ab initio* method was used in [5], therefore here and further data are given by me in the interpretation of MNDO and ZINDO / 1

From the heteroatoms of alanine and valine, one can observe, is smallest outflow of charge (during the formation of ironcomplexes), which is explained by the primitivity of variable part of R. The protective effects of corrosion of these amino acids are also close.

The highest charge outflow (during the formation of ironcomplexes) is carried out by tryptophan and phenylalanine (a large variable part of R). The spread of protective effects of corrosion is greater.

Table 2.

THE VALUES OF THE CALCULATED QUANTUM CHEMICAL DESCRIPTORS OF AMINO ACIDS OF SKELETON II AND COMPLEX COMPOUNDS BASED ON IT

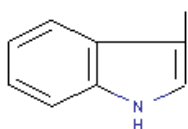
Codes of corrosion inhibitors	THR	ALA	VAL
Σq	-1.244	-0.930	-0.919
Partial effective charges on heteroatoms	${}^6q_O = -0.313$	${}^2q_N = -0.267$	${}^2q_N = -0.264$
	${}^7q_O = -0.298$	${}^5q_O = -0.311$	${}^6q_{CH_3} = -0.018$
	${}^8q_O = -0.368$	${}^6q_O = -0.352$	${}^7q_O = -0.313$
	${}^2q_N = -0.265$		${}^8q_O = -0.342$
Empirical formulas of $Fe_x \leftarrow AA$	$Fe_{10} \leftarrow THR$	$Fe_8 \leftarrow ALA$	$Fe_{11} \leftarrow VAL$
Σq	-0.468	-0.354	-0.261
Partial effective charges on heteroatoms	${}^6q_O = -0.142$	${}^2q_N = -0.136$	${}^2q_N = -0.095$
	${}^7q_O = -0.072$	${}^5q_O = -0.094$	${}^6q_{CH_3} = 0.000$
	${}^8q_O = -0.137$	${}^6q_O = -0.124$	${}^7q_O = -0.051$
	${}^2q_N = -0.116$		${}^8q_O = -0.115$
$Fe\rho_q$	-0.307	-0.304	-0.299

Table 3.

THE VALUES OF THE CALCULATED QUANTUM-CHEMICAL DESCRIPTORS OF AMINO ACIDS OF SKELETON III AND COMPLEX COMPOUNDS BASED ON IT

Codes of corrosion inhibitors	TRP	TYR	PHE
Σq	-1.398	-1.428	-1.281
Partial effective charges on heteroatoms	${}^2q_N = -0.269$	${}^2q_N = -0.266$	${}^2q_N = -0.267$
	${}^{14}q_O = -0.289$	${}^9q_O = -0.245$	${}^{11}q_O = -0.311$
	${}^{15}q_O = -0.375$	${}^{12}q_O = -0.284$	${}^{12}q_O = -0.349$
	${}^7q_N = -0.236$	${}^{13}q_O = -0.374$	$Benz\Sigma q = -0.354$
	$Benz\Sigma q = -0.229$	$Benz\Sigma q = -0.259$	
Empirical formulas of $Fe_x \leftarrow AA$	$Fe_{12} \leftarrow TRP$	$Fe_{12} \leftarrow TYR$	$Fe_{13} \leftarrow PHE$
Σq	0,914	0,803	1,014
Partial effective charges on heteroatoms	${}^2q_N = -0.132$	${}^2q_N = -0.154$	${}^2q_N = -0.156$
	${}^{14}q_O = -0.052$	${}^9q_O = -0.140$	${}^{11}q_O = -0.049$
	${}^{15}q_O = -0.160$	${}^{12}q_O = -0.149$	${}^{12}q_O = -0.105$
	${}^7q_N = -0.025$	${}^{13}q_O = -0.160$	$Benz\Sigma q = 1.324$
	$Benz\Sigma q = 1.283$	$Benz\Sigma q = 1.406$	
$Fe\rho_q$	-0.415	-0.382	-0.347

In cysteine there are atoms of sulfur and nitrogen, which have strong donor properties (Tables 1–3). In amino acids of Skeleton II, valine contains a strongly-donor nitrogen atom, which makes the greatest contribution to inhibition due to non-polarity *R*. In the amino acids of Skeleton III, the nitrogen atom is weaker as a donor, only the nitrogen atom is a strong donor in the composition of



— ring, since the electron pair of 7N has a +M-effect to a lesser degree than, for example, in the aniline molecule.

Consequently, the larger and more polar of *R* radical, the lesser need for donor properties of nitrogen atom of main carbon chain.

Oxygen atoms are very strong as donors (of which the oxygen atoms of keto groups are the most potent as donors, as you will see from tables 4–9) in Skeleton I (serine and aminobutanoic acid), in Skeleton II and Skeleton III (tryptophan and phenylalanine).

The highest Z% are achieved due to the presence of benzene (Benz) rings in Skeleton III up to the recharging of benzene rings (charge exchange is smallest in tyrosine apparently due to the additional introduction of an electron pair from the oxygen atom of phenolic hydroxyl).

In the composition of complex compounds, the x is inversely proportional to the inhibition efficiency exhibited by these amino acids.

Values of the energy of boundary orbitals. Energy diagrams.

Values and changes in the energies of boundary orbitals inside AA and inside $Fe_x \leftarrow AA$ are shown in diagrams 1–3. The magnitudes and signs of values of boundary orbitals are the most common for characterizing donor and acceptor properties of molecules, according to [32–36]:

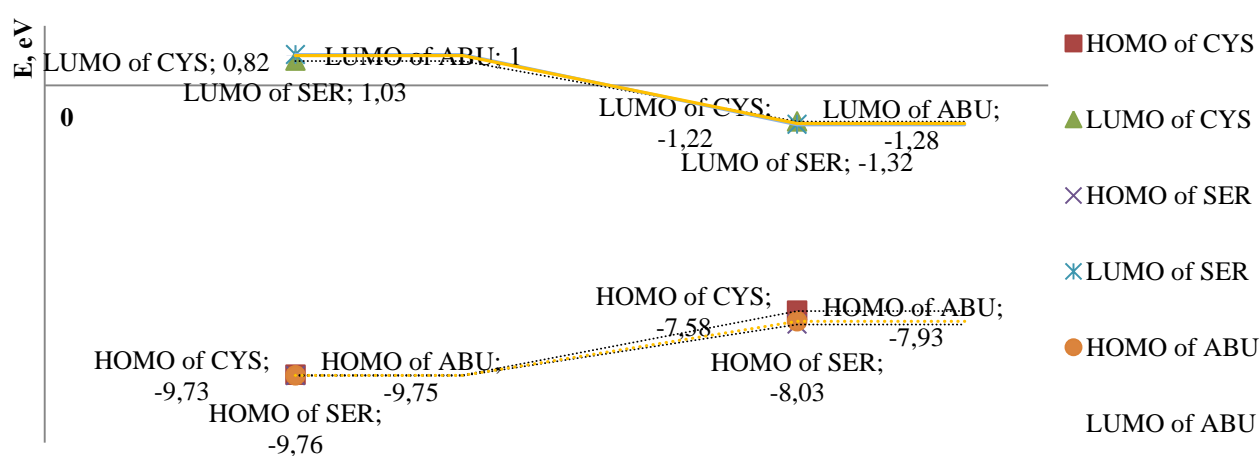


Figure 1. The energies of boundary orbitals inside $Fe_x \leftarrow AA$ of Skeleton I (in the right position) and inside AA of Skeleton I (in the left position)¹

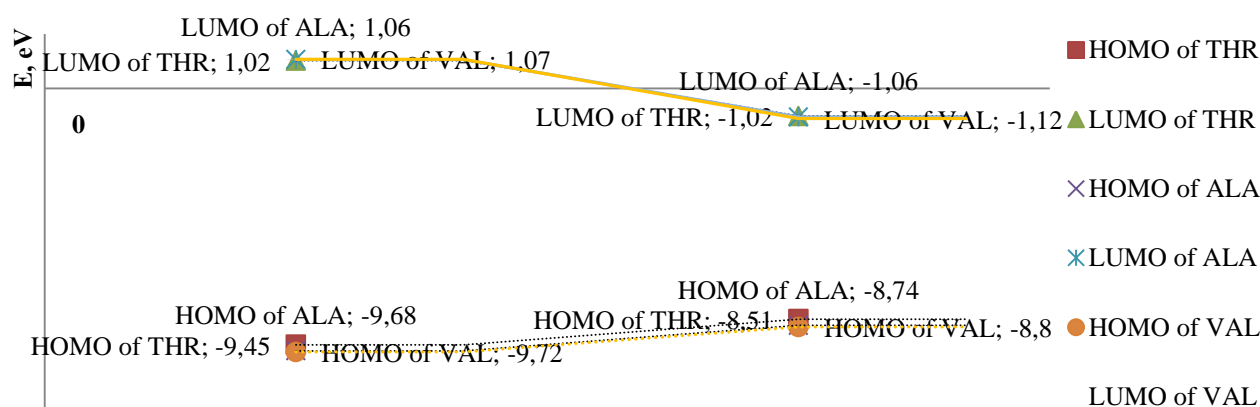


Figure 2. The energies of boundary orbitals inside $Fe_x \leftarrow AA$ of Skeleton II (in the right position) and inside AA of Skeleton II (in the left position)

¹ Diagrams 1-3 in the left-hand position show the energies of boundary orbitals of the original molecules from [5] that are in the gas phase

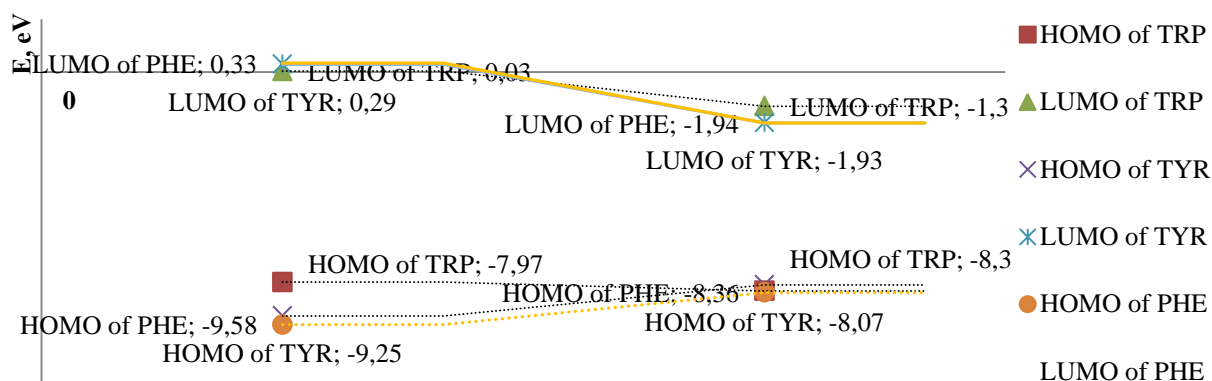


Figure 3. The energies of boundary orbitals inside $Fe_x \leftarrow AA$ of Skeleton III (in the right position) and inside AA of Skeleton I (in the left position)

With help of Diagrams 1–3 there is a possibility, in the author's opinion, to evaluate the strengths of $Fe_x \leftarrow AA$ adsorption complexes that are capable of degradation in the acid corrosive medium created by 0,01 M H_2SO_4 . The oxidation (it is $Fe^0 - 2e = Fe^{2+}$) can occur [5, 6, 15, 16, 18, 20, 21, 23, 24, 27–32, 35]. The destruction of $Fe_x \leftarrow AA$ appears because with the formation of $Fe_x \leftarrow AA$ the ionization energy I decreases.

In the $Fe_{12} \leftarrow TRP$, on the contrary, there is an increase of I , so this complex will be most stable in an acidic corrosive environment. Also, there are high donor properties of tryptophan. Therefore, there is a high $Z\%$.

Graphical dependencies

Dependence between the charge density per iron atom and the inhibition efficiency for a Skeleton I and III

Dependence between the $Z\%$ in 0.01 M and in 0.02 M of inhibitor concentration and the charge density per iron atom is follows (Figure 4), but it is possible to build only for Skeleton I and III (with a measurable angle value):

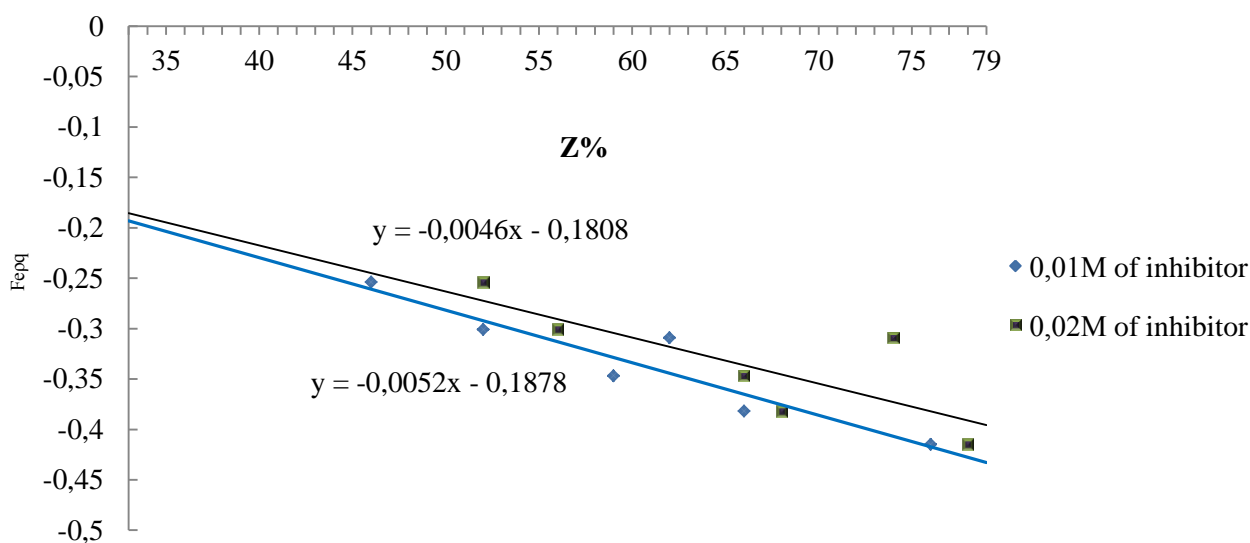


Figure 4. Graphical dependence of the type " $Fe\rho_q$ — $Z\%$ " in selected concentrations

As the concentration of inhibitor increases, the “concentration” of heteroatoms increases in corrosive system, so high Z% is reached at a lower charge density per iron atom. Or, the molecules of the adsorbed corrosive medium are replaced by the inhibitor molecules on the metal "surface" (adsorption of corrosive medium also determines the Z% value).

Dependence between the energy of the higher filled molecular orbital of ironcomplex and the inhibition efficiency for a Skeleton II

For Skeleton II, the most convenient — instead of $F_{Fe\rho q}$ — is to take the energy of higher occupied molecular orbital of ironcomplexes (since the angle will be larger), this is shown in Figure 5:

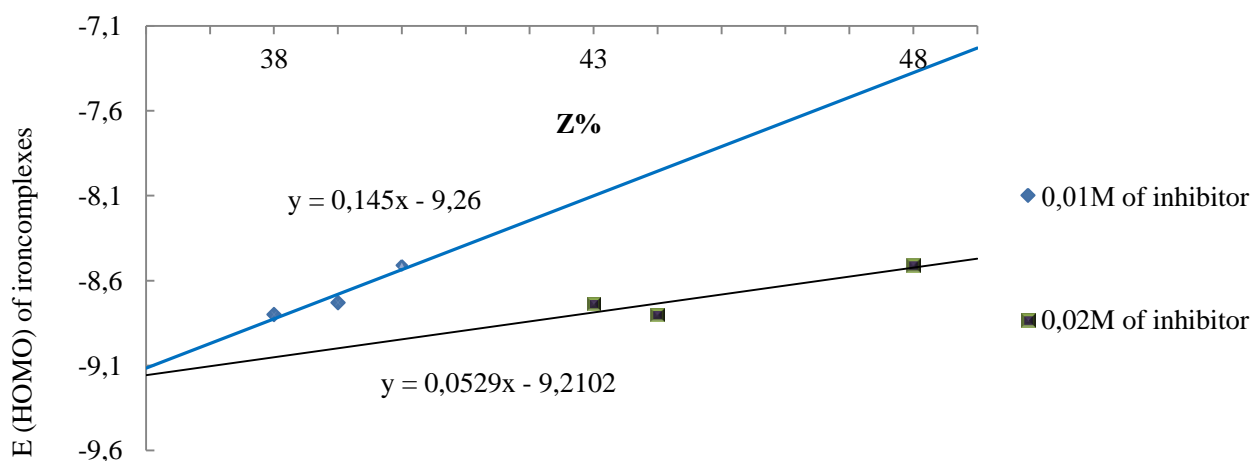


Figure 5. Graphical dependence of the type “E (HOMO) of ironcomplexes — Z%” in the selected concentrations

With increasing concentration, Z% most sharply increases.

The increase in energy of the higher filled molecular orbital gives better inhibitory properties of amino acids at a 0.01 M of inhibitor concentration.

At a 0.02 M of concentration, the graphical dependence shows a smaller angle, which means that the ionization energy plays a lesser role in the inhibition efficiency in this corrosive medium.

The ironcomplexes

Characterization of donor and acceptor bonds

Values of valence listed in Tables 4–9 and it is "joint activity" of heteroatoms radius and the strength of ligands electronic field capable of capturing electron-deficient iron atoms (iron atoms are Lewis acids; amino acids are Lewis bases).

Table 4.

THE LENGTHS OF DONOR AND ACCEPTOR BONDS IN Fe₈ ← CYS

<i>The charge of the iron atom</i>	<i>The chemical bond of an iron atom with a specific adsorption center</i>	<i>Length of chemical bond, Angstrom</i>
-0.321	Fe ₋₂ N	2.50
-0.316	Fe ₋₂ N	2.44
	Fe ₋₆ O	2.38
	Fe ₋₇ O	2.45
-0.493	Fe ₋₆ O	2.27
-0.276	Fe ₋₆ O	2.26
-0.234	Fe ₋₆ O	2.42
	Fe ₋₇ O	2.30
-0.396	Fe ₋₅ S	2.65
-0.287	Fe ₋₅ S	2.50
-0.146	Fe ₋₅ S	2.50

Table 5.

THE LENGTHS OF DONOR AND ACCEPTOR BONDS IN Fe₉ ← SER

<i>The charge of the iron atom</i>	<i>The chemical bond of an iron atom with a specific adsorption center</i>	<i>Length of chemical bond, Angstrom</i>
-0.296	Fe ₋₂ N	2.40
-0.308	Fe ₋₂ N	2.47
	Fe ₋₆ O	2.38
-0.301	Fe ₋₆ O	2.21
-0.224	Fe ₋₆ O	2.24
-0.360	Fe ₋₇ O	2.25
-0.317	Fe ₋₅ O	2.37
-0.229	Fe ₋₅ O	2.30
-0.293	Fe ₋₅ O	2.34
-0.175	Fe ₋₅ O	2.70

Table 6.

THE LENGTHS OF DONOR AND ACCEPTOR BONDS IN Fe₉ ← ABU

<i>The charge of the iron atom</i>	<i>The chemical bond of an iron atom with a specific adsorption center</i>	<i>Length of chemical bond, Angstrom</i>
-0.297	Fe ₋₇ N	2.40
	Fe ₋₆ O	2.50
	Fe ₋₅ O	2.42
-0.452	Fe ₋₅ O	2.46
-0.428	Fe ₋₅ O	2.25
-0.237	Fe ₋₅ O	2.16
	Fe ₋₄ N	2.38
-0.317	Fe ₋₆ O	2.19
-0.247	Fe ₋₄ N	2.70
-0.129	Fe ₋₄ N	2.27
-0.283	Fe ₋₄ N	2.34
-0.314	Fe ₋₇ N	2.35

Analyzing the content of Tables 4–6 and constructing the SER → ABU → CYS series, one can find the following: 1) the oxygen atoms of the keto groups are most active as electron density donors, since they have a higher denticity. 2) According to the donor properties of R, the oxygen atom is worst donor, the sulfur atom is the best donor in full accordance with [2]. 3) there is a slight increase in the average valence of iron atoms. 4) the correlation "Z% / bond length Fe-adsorption center" is not revealed.

Table 7.

THE LENGTHS OF DONOR AND ACCEPTOR BONDS IN Fe₁₂ ← TRP

<i>The charge of the iron atom</i>	<i>The chemical bond of an iron atom with a specific adsorption center</i>	<i>Length of chemical bond, Angstrom</i>
-0.296	Fe- ₂ N	2.77
-0.564	Fe- ₁₄ O	2.46
-0.592	Fe- ₁₄ O	2.30
	Fe-Benz	1.99
-0.492	Fe- ₂ N	2.23
-0.263	Fe- ₁₄ O	2.31
	Fe- ₁₅ O	2.35
-0.607	Fe- ₁₄ O	2.30
	Fe- ₁₅ O	2.38
-0.266	Fe- ₉ C	2.43
-0.315	Fe- ₇ N	2.31
-0.225	Fe- ₁₀ C	2.40
-0.446	Fe- ₁₃ C	2.44
	Fe- ₅ C	2.30
	Fe- ₆ C	2.27
-0.562	Fe- ₁₄ O	2.28
-0.395	Fe- ₂ N	2.31
	Fe- ₁₅ O	2.20
-0.574	Fe-Benz	1.82

Table 8.

THE LENGTHS OF DONOR AND ACCEPTOR BONDS IN Fe₁₂ ← TYR

<i>The charge of the iron atom</i>	<i>The chemical bond of an iron atom with a specific adsorption center</i>	<i>Length of chemical bond, Angstrom</i>
-0.246	Fe- ₂ N	2.21
-0.457	Fe- ₂ N	2.24
	Fe- ₁₂ O	2.24
-0.340	Fe- ₁₂ O	2.37
-0.205	Fe- ₁₂ O	2.21
-0.386	Fe- ₁₃ O	2.31
-0.441	Fe- ₁₃ O	2.24
-0.588	Fe- ₁₃ O	2.43
	Fe-Benz	1.90
-0.313	Fe- ₇ C	2.39
-0.310	Fe- ₁₀ C	2.40
-0.304	Fe- ₆ C	2.37
-0.418	Fe- ₆ C	2.44
-0.395	Fe- ₂ N	2.31
	Fe- ₁₅ O	2.20
-0.580	Fe-Benz	1.90

Table 9.

THE LENGTHS OF DONOR AND ACCEPTOR BONDS IN Fe₁₃ ← PHE

<i>The charge of the iron atom</i>	<i>The chemical bond of an iron atom with a specific adsorption center</i>	<i>Length of chemical bond, Angstrom</i>
-0.336	Fe- ₂ N	2.24
	Fe- ₁₂ O	2.28
-0.267	Fe- ₁₁ O	2.50
-0.223	Fe- ₁₁ O	2.24
-0.650	Fe- ₁₁ O	2.47
	Fe-Benz	1.89
-0.473	Fe- ₁₂ O	2.31
-0.500	Fe- ₁₁ O	2.31
-0.200	Fe- ₉ C	2.43
-0.235	Fe- ₇ C	2.39
-0.201	Fe- ₈ C	2.50
-0.188	Fe- ₉ C	2.46
-0.500	Fe- ₁₀ C	2.33
-0.318	Fe- ₆ C	2.46
-0.351	Fe- ₂ N	2.40
-0.575	Fe-Benz	1.95

Analyzing the content of Tables 7–9 and building a series of PHE → TYR → TRP, one can observe the following: 1) a sharp increase in the average valency of iron atoms. 2) an inaccurate increase in the dentacy of nitrogen atom. 3) growth of dentateness of hydroxyl oxygen atom from tyrosine to tryptophan. 4) decrease in the distance from the iron atoms belonging to the benzene ring to the benzene ring. 5) the oxygen atom in the tryptophan radical has no connection with the iron atoms; in the phenylalanine molecule it is absent; in the tryptophan molecule, the ₇N atom exhibits a dentacy of 1. 6) In benzene rings, phenylalanine and tyrosine molecules attract the most iron atoms. 7) the correlation "Z% / bond length "Fe-adsorption center" is not revealed.

Conclusion

The approximations used in this paper, such as the absence of hydration of the molecule, the neglect of the inevitable adsorption of molecules of the corrosive medium on the metal, semiempirical methods of modeling and calculation obviously allow one to obtain the predictive power of the improved theory of cluster modeling. This improvement provides more information about the protection of metal inhibitors than traditional and conventional theory. An improved method of quantum-chemical modeling provides a much more complete set of data that can serve as an effective predictive tool than traditional and conventional theory, much less the "structure-property" correlation method [31–36] due to the abandonment of the preliminary surface problem metal. Since iron complexes are not considered as surface compounds but are considered as independent chemical compounds (or rather an adduct) with a clearly defined chemical composition, analogous to well-known π-complexes, it is possible to trace the initial and final state of the ligand molecule, the adsorbed organic compound. This is fraught with great promise, because at present, the selection of inhibitors corrosion is increasingly carried out with quantum-chemical prediction methods [32–36] rather than by the method of the past years and decades (the screening).

There is no doubt that the development of new quantum–chemical programs versions, basic sets, and the development of visualization software play a significant role in shaping the improvements in quantum–chemical modeling. Increasingly productive computers often become an indispensable attribute of any area of the economy and the national economy, traditional approaches to the problem of inhibiting corrosion will be less necessary, along with an increase in the level of quantum–chemical theory.

Competing interests

The authors declare that they have no competing interests.

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