ХИМИЧЕСКИЕ НАУКИ / CHEMICAL SCIENCES

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STUDY OF SULFONAMIDES (USED AS CORROSION INHIBITORS) FOR POSSIBILITY TO ADSORPTION ON STEEL

ИНГИБИРОВАНИЕ МИКРОБИОЛОГИЧЕСКОЙ СЕРОВОДОРОДНОЙ КОРРОЗИИ ОРГАНИЧЕСКИМИ ПРОИЗВОДНЫМИ НА ОСНОВЕ БЕНЗОЛСУЛЬФАМИДА

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Abstract: In this paper, the process of adsorption of organic compounds of the sulfonamides class on iron (available in 97% of St3 steel) is modeled using the HyperChem package version 8.0.7 using the semi–empirical ZINDO / 1 method. The structures of sulfonamides for the study were chosen so that the sequential complication of the molecular structure could be traced. Such an approach, as will be shown below, accurately reflects the process of corrosion protection with bacterial content by chemisorption of an organic compound on the metal surface to form a complex compound. In the course of the study, the compositions of the complexes obtained, the energies of the boundary orbitals, and a graph depicting the dependence of the charge density on the iron atom on the component of the corrosion rate that is due to chemisorption effects were obtained and analyzed. On the graph there are equations of lines.

Аннотация. В публикуемой работе представлен смоделированный посредством квантовохимического пакета HyperChem версии 8.0.7 используя полуэмпирический метод ZINDO/1 процесс адсорбции органических соединений класса сульфаниламидов, на железе (имеющегося в стали Ст3 в количестве 97%). Структуры сульфаниламидов для исследования были выбраны так, чтобы прослеживалось последовательное усложнение молекулярной структуры. Такой подход, как будет показано далее, с высокой точностью отражает процесс защиты от коррозии с бактериальным контентом путем хемосорбции органического соединения на поверхности металла с образованием комплексного соединения. В процессе исследования были получены и проанализированы: составы полученных комплексов, энергии граничных орбиталей, график, отображающий зависимость плотности заряда, приходящегося на атом железа, от той составляющей скорости коррозии, которая обусловлена хемосорбционными эффектами. На графике показаны уравнения прямых.

Keywords: sulfonamides, corrosion rate, sulfate–reducing bacteria, hydrogen sulfide corrosion, chemical adsorption, St3 steel, iron, partial effective charges, molecule rigidity, electronegativity of the molecule, global electrophilicity of the molecule, composition of complex compounds.

Ключевые слова: сульфаниламиды, скорость коррозии, сульфатредуцирующие бактерии, сероводородная коррозия, химическая адсорбция, сталь Ст3, железо, парциальные эффективные заряды, жесткость молекулы, электроотрицательность молекулы, глобальная электрофильность молекулы, состав комплексных соединений.

Systematization of data on the inhibitory effect of various SMs (this is the test compound) allowed many scientists (both Soviet–Russian and foreign) to reveal many patterns in the structure of the compound that give it properties that inhibit hydrogen sulphide corrosion. First of all, such a property depends on the presence of heteroatoms in the structure of SM, since the deposition of free electron pairs allows such compounds to dose the electron density to unfilled *d*–orbital of the metal (in the case of mild steel, these sublevels are *3d*), giving surface complexes that to some extent inhibit Cathodic and anodic reaction of electrochemical corrosion involving hydrogen sulphide. As a consequence, a decrease in the corrosion rate should be observed. In our study, such hetero–atoms are nitrogen, oxygen, sulfur, the former having a smaller electronegativity, which is regarded in [1, 8, 13] as a good and useful feature.

Unlike chelating agents (for example, EDTA), for which only chemisorption inhibitory microbiological corrosion action was described by outside authors, there is colossal evidence for their benzene sulfonamide derivatives specifically for their antimicrobial activity (as studies of the 1930s on the inhibition of streptococcus, gonococcus, meningococcus, pneumococcus, Staphylococcus, E. coli, etc., and a study of a decrease in the titer of nonpathogenic sulfate–reducing bacteria, performed in the Kaliningrad State University (Kaliningrad, Russian Federation) in 2004) [22]. In contrast to chelating agents (for example, EDTA) for which the chemisorption inhibiting microbiological corrosion action depends on the presence of heteroatoms and (in part) on the chelating effect, for the benzenesulfonamide derivatives, the inhibitory bacterial titre depends on the presence of the amino group (or amino group derivatives which generate, during hydrolysis, the amino group) in the *4*-position of cycle A (view further in the text).

The scientific novelty of the study is a departure from the cluster modeling technology and the attraction of a more informative approximation of the donor–acceptor interaction of SM with iron atoms (which is a good approximation, since 97% of iron is present in St3S steel), so the author finds the possibility of introducing the concept of " ($_{Fe}\rho_q$ is the charge per iron atom (charge density)), which has the same dimension as the value of the partial effective charge. The author believes that this value can become an alternative to the degree of charge transfer ΔN [21]. As will be shown later, this SM characteristic is linearly dependent on the corrosion rate in a hydrogen sulfide medium with the presence of sulfate–reducing bacteria cells. Thus, it is possible to detect the most important centers of chemical adsorption, as will be shown later also.

Methods

A variety of microbiological corrosion system.

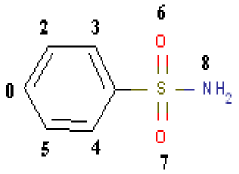
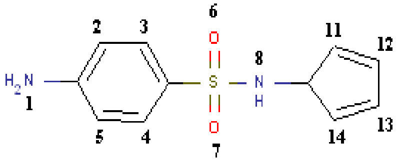
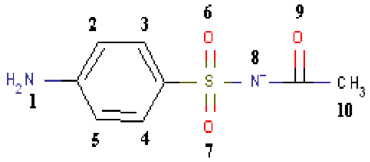
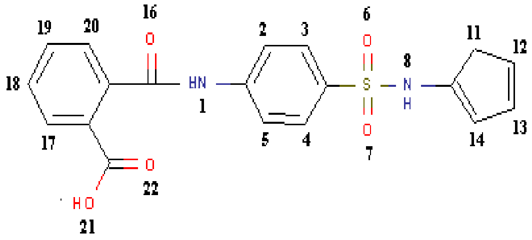
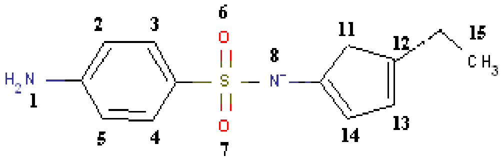
In the article investigated the heterogeneous thermodynamic system of closed type “St3S+ sulfate–reducing bacteria cells”. Samples of steel were parameters 20×50×1 mm.

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

Five representatives of the sulfonamide class were selected on the basis of a sequential complication of their structure compared with the “original” (SM 1). The corrosion rate data were taken from [22] for 5 representatives of the sulfonamide class, acting as inhibitors of hydrogen sulfide corrosion, added at a concentration of 1, 2, 10 mmol / l contained in a closed system (this is a tube with a volume of 0.9 L) Liquid sterile de–oxygenated medium Postgate “B” (Table 1).

Table 1.

USEFUL OF ORGANIC COMPOUND FOR INHIBITORS

Abbreviation of inhibitor	*Structural formulas with numbered (according to the author, not according to IUPAC) assumed adsorption centers*	*Preferred IUPAC name of inhibitor*	*Molecular weight*
SM 1		Benzene-sulfonamide	157,1
SM 2		4-amino-N-(cyclopenta-2,4-dien-1-yl)benzene-1-sulfonamide	236.3
SM 3		Acetyl[(4-aminobenzene)sulfonyl]azanide	213.2
SM 4		2-({4-[(cyclopenta-1,3-dien-1-yl)sulfamoyl]phenyl}carbamoyl)benzoic acid	384.4
SM 5		4-{[(4-ethylcyclopenta-1,3-dien-1-yl)azanidyl]sulfonyl}aniline	263.3

These SMs were synthesized at the Department of Organic Chemistry of Tambov State University (Tambov, Russian Federation) with guidance of Professor Sergey M. Beloglazov.

The technology of experiment

The technology of carrying out a numerical experiment consisted in setting the limiting number of iron atoms, which was considered to be their number *a*, when the number *b* of zero atoms was transferred from *(a + b)* of given iron atoms. Then it was assumed that the donor capabilities of SM were exhausted. The plane of neutral iron atoms specified by the user of HyperChem was 1,2 A away from the SM plane with the expectation that the program produced fewer iterations, which provides the necessary accuracy. The equation for the electrophilic reaction was as follows: $x\mathrm{Fe}^0 + \mathrm{SM\ Y} = \mathrm{Fe}_x \leftarrow [\mathrm{SMY}]$. The latter according to the generally accepted classification should be classified as complex, since there is a presence of donor–acceptor interactions, where the iron atoms are acceptors, which in this connection are negatively charged. Along the length of “*Fe–heteroatom*” bond was taken into account within the 2,50 angstroms (A).

The technology of quantum chemical calculations

The data was calculated using HyperChem 8.0.7. The determination of the quantum chemical descriptors was carried out in two stages: by optimizing the geometry by the molecular mechanics method: first MM +, and then OPLS. The actual calculation was carried out within the framework of ZINDO / 1 [2, 10]. When specifying the source structure, the mesomeric effect of the SM chain was taken into account in the job–file. It follows from Table 1 that the cyclic conglomerate formed by carbon atoms 11–14 in SM 4 and SM 5 enters the global chain of mesomerism (in contrast to that in SM 2, so we can conclude that the structures and properties of SM 2 and SM 3. Although, the anion center in the structure of SM 3 debunks the illusion). The following descriptors of the electron structure were monitored: charges on the heteroatoms of metalloids (according to R. Mulliken), the energy of the boundary orbitals, and also the composition of the resulting compounds of the Fe_x ← [SM Y] type, where SM acts as a ligand. The values of the quantum–chemical descriptors will be presented and discussed below.

Results and discussion

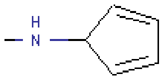
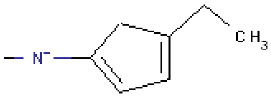
The generated results are summarized in Table 2. The values of the stiffness of the molecules η, of the electronegativity (chemical potential of the molecule) χ, of the global electrophilicity I_E will be calculated from the formulas [16–18].

Table 2.

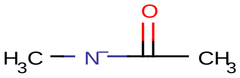
THE VALUES OF THE CALCULATED QUANTUM–CHEMICAL DESCRIPTORS
OF MOLECULES OF SULFONAMIDES AND COMPLEX COMPOUNDS BASED ON THEM

Codes of inhibitors	*SM 1*	*SM 2*	*SM 3*	*SM 4*	*SM 5*
1	*2*	*3*	*4*	*5*	*6*
η	15,324	13,602	12,396	9,248	10,909
χ	1,672	0,957	−4,327	−0,548	−5,291
$\mathbf{I_E}$	0,0912	0,0337	0,755	0,0162	1,283
Partial effective charges on atoms	$q_S = 0,560$	${}_1q_N = -0,338$	${}_1q_N = -0,344$	${}_{16}q_O = -0,145$	${}_8q_N = -0,427$
	${}_7q_O = -0,408$	$q_S = 0,534$	$q_S = 0,477$	${}_1q_N = -0,238$	$q_S = 0,473$
	${}_6q_O = -0,419$	${}_7q_O = -0,419$	${}_6q_O = -0,480$	$q_S = 0,548$	${}_7q_O = -0,476$
	${}_8q_N = -0,306$	${}_6q_O = -0,431$	${}_7q_O = -0,481$	${}_7q_O = -0,415$	${}_6q_O = -0,475$
		${}_8q_N = -0,234$	${}_8q_N = -0,420$	${}_6q_O = -0,420$	${}_1q_N = -0,345$
			${}_9q_O = -0,554$	${}_8q_N = -0,224$	
Composition of adsorption complexes	Fe_{10}← SM1	Fe_{15}← SM2	Na^+Fe_{18}←SM3 ¯	Fe_{19}← SM4	Na^+Fe_{19}← SM5¯
η	5,621	5,013	5,379	6,099	6,113
χ	5,055	5,481	2,208	4,855	2,063
$\mathbf{I_E}$	2,273	3,004	0,453	1,932	0,348
Partial effective charges on atoms	$q_S = 0,766$	${}_1q_N = -0,136$	${}_1q_N = -0,109$	${}_{16}q_O = -0,029$	${}_{ca}q_N = -0,038$
	${}_7q_O = -0,029$	$q_S = 0,785$	$q_S = 0,782$	${}_1q_N = -0,127$	$q_S = 0,800$
	${}_6q_O = -0,036$	${}_7q_O = -0,040$	${}_6q_O = -0,033$	$q_S = 0,765$	${}_1q_O = -0,035$
	${}_8q_N = -0,111$	${}_6q_O = -0,069$	${}_7q_O = -0,020$	${}_7q_O = -0,015$	${}_2q_O = -0,033$
		${}_8q_N = -0,076$	${}_8q_N = -0,028$	${}_6q_O = -0,057$	${}_6q_N = -0,133$
			${}_9q_O = -0,083$	${}_8q_N = -0,034$	
$\mathbf{{}_{Fe}\rho_q}$	−0,296	−0,397	−0,300	−0,445	−0,398

The studied molecules belong to the class of rigid reagents, with a hard–to–polarize electron pair at the HOMO [4, 11, 12].

Adsorption compounds are soft reagents according to the Pearson's theory, this property is attached to adsorbed iron atoms. Also, in the formation of these complexes, there is a sharp increase in the electronegativity χ and the global electrophilicity I_E (except for SM 5 and SM 3). In SM 5 and SM 3, I_E declines, this occurs in SM 5 most dramatically. In SM 5, a less powerful anionic center, since the delocalization of the electron density from this anion center proceeds both to the *4-sulfonyl}aniline* ring and to *4-ethylcyclopenta-1,3-dien-1-yl*. In SM 3, delocalization is one–sided, only *4-aminobenzene)sulfonyl*, therefore, in the presence of SM 3, the corrosion rate decreases approximately as in the presence of SM 1. In SM 4, the anion center on the $_{21}$O and $_{22}$O atoms does not appear to prevents the inhibition of corrosion, since its area is small compared to the area of a large SM 4. Also, the benzene ring **C** (also in conjugation with an electron–withdrawing group of $_{16}$O) effectively delocalizes the anionic center. In SM 2, there is no anionic center and the electron pair strength at $_8$N in the group of atoms  is the same as in the group of atoms  (SM 5). This explains the same charge density at the iron atom.

In the case of SM 1 (there is no $-NH_2$ anionic center) and SM 3 is the electron pair strength at $_8$N in the group of atoms_and is the same as in the group of atoms



$H_3C-N^{-}-\overset{O}{\|}-CH_3$

[23].

More interesting is the presence of charges on heteroatoms. The charges q_S are of interest as a characteristic of electrosorption. They are long, their length is over 2.5A. The charges q_S are positive, when the interaction xFe + SM Y = $Fe_x \leftarrow$ [SM Y] their values increase. This shows that they play a role in the process of physical adsorbing, and the growth of charge is explained by the outflow of electron density to iron atoms, and then from the benzene ring to sulfur and carbon atoms. The growth of the charge in connection with these one–time processes by means of coupling through the $S^{\delta+} \rightarrow Fe^{\delta-}$ bonds enhances the electro sorption.

The remaining charges are negative modulo. This is naturally their increase in compounds of the composition $Fe_x \leftarrow$ [SM Y], which is explained by the donor–acceptor interaction with iron (chemical adsorption) [3, 5–7].

The dependence of the corrosion rate in the inhibitor concentration of 1, 2, 10 mmol / L on the charge density on iron $_{Fe}\rho_q$ is expressed graphically (using linear trend lines) as follows (see Figure 1).

If the graphical dependence were parallel, it would mean that there is no chemisorption component in the effect of inhibiting microbiological corrosion. It is obvious that at a concentration of 1 mmol / L such a dependence is most similar to that at a concentration of 2 mmol / L. A sharper increase in density leads to a sharper decrease in the rate of corrosion. At higher concentrations, such a relationship persists, but is less pronounced. The dependence of the corrosion rate on the charge density on the iron is not lost at an inhibitor concentration of 1 mmol / L, but it can be lost at 2 and 10 mmol / L in the case of a corrosion rate of 2.5.

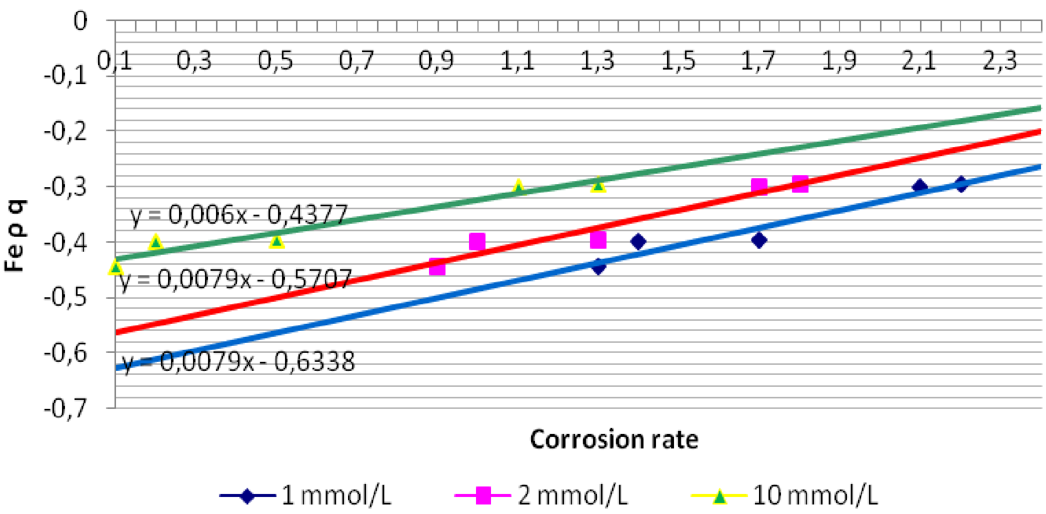


Figure 1. Dependence of corrosion rate and charge density on iron

The mesomeric effect manifests itself over the whole area of the molecule in SM 1, SM 4, SM 5. In the adsorption complexes Fe_x ← [SM Y], the electron density cannot “blur” with the same ease with which it was in SM Y. Iron atoms ‘sew’ the electron density at fixed places. This explains the symmetrical distribution of partial effective charges on heteroatoms, the symmetrical distribution of the charges of iron atoms on both sides of the benzene ring and the distances from these iron atoms to the benzene ring plane. In the adsorption complexes Fe_x ← [SM Y] there is a coordination number of iron I ... III.

Tables 3–7 describe the structures of the adsorption complexes formed. Obviously, the value of Feρq (depending on the structural similarity of the complexes) is dependent on the number of iron atoms — for each iron atom, an increase of $_{Fe}\rho_q$ by −0,020 on average is necessary. If there is an anion center in the structure of SM, the value of $_{Fe}\rho_q$ increases by −0,100 on average. Naturally, this is an empirical regularity. The magnitudes of the valences indicated in Tables 3–7 are formed on the basis of the “joint activity” of the radius of heteroatoms and the strength of the electron density of the electron density capable of capturing electron–deficient iron atoms.

Table 3.

LENGTHS OF DONOR–ACCEPTOR BONDS IN Fe_{10} ← [SM1]

The charge of a particular iron atom	*Name of bonds with heteroatom*	*quantum chemically calculated length relationships, A*
1	*2*	*3*
−0,305	Fe–$_2$C Fe–$_0$C	2,37 2,32
−0,377	Fe–$_3$C Fe–$_6$O	2,38 2,34
−0,227	Fe–$_6$O	2,27

End Table 3.

1	2	3
−0,205	Fe–$_6$O Fe–$_7$O	2,35 2,37
−0,271	Fe–$_8$N Fe–$_7$O	2,38 2.45
−0,377	Fe–$_7$O Fe–$_3$C Fe–$_6$O	2,50 2.41 2.48
−0,426	Fe–$_3$C Fe–$_8$N	2,42 2,17
−0,394	Fe–$_7$O Fe–$_4$C	2,45 2,37
−0,573	Fe–A[1]	2,22
−0,568	Fe–A	2,22

In Fe_{10} ← [SM1], the greatest contribution to the charge density on the iron atom (hence, to inhibition of corrosion) gives $_6$O, also $_7$O and $_3$C. The dentateness of the SM 1 as a ligand over the nitrogen atom is II, in total, oxygen atoms are VIII (this is IV for $_6$O and $_7$O).

Table 4.

LENGTHS OF DONOR–ACCEPTOR BONDS IN Fe_{15} ← [SM 2]

The charge of a particular iron atom	*Name of bonds with heteroatom*	*quantum chemically calculated length relationships, A*
1	*2*	*3*
−0,268	Fe–$_5$C	2,40
−0,199	Fe–$_5$C Fe–$_4$C	2,49 2,49
−0,318	Fe–$_1$N	2,21
−0,389	Fe–$_8$N Fe–$_7$O	2,50 2,26
−0,174	Fe–$_6$O Fe–$_7$O	2,34 2.26
−0,461	Fe–$_6$O Fe–$_8$N Fe–$_{11}$C	2,37 2.34 2.45
−0,296	Fe–$_{12}$C	2,30
−0,285	Fe–$_{13}$C Fe–$_{14}$C	2,36 2,42
−0.369	Fe–$_3$C Fe–$_7$O	2.48 2.35
−0.305	Fe–$_6$O Fe–$_4$C	2.29 2.50
−0.349	Fe–$_1$N Fe–$_2$C Fe–$_8$N	2.24 2.42 2.34

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[1] iron atoms are grouped in 2 mutually parallel planes, which are also parallel to the plane of the cycles in the molecules under study, the letters mean: A is a cycle consisting of carbon atoms 2–5, B is a cycle of carbon atoms 11–14, C is a ring of carbon atoms 17–20

End Table 3.

1	*2*	*3*
−0.757	$Fe–_8N$	2.34
−0.757	Fe–A	2.42
−0.568	Fe–A	2.36
−0.555	Fe–B	2.04
−0.658	Fe–B	1.96

In Fe_{15} ← [SM2], the dentacy of the test compound as a ligand on the nitrogen atom is IV (II there is for $_1N$ and II there is for $_8N$), in total oxygen atoms are VI (III there is for $_6O$ and III there is for $_7O$), which is associated with an increase in the area of the molecule–ligand. The greatest contribution to the inhibition of corrosion is provided by the $_8N$, $_6O$ and $_7O$ atoms. The absence of a mesomeric effect over the entire area of the molecule does not give a symmetrical distribution of charges on the corresponding iron atoms, and also distances to the plane of the cycle are practically equal.

Table 5.

LENGTHS OF DONOR–ACCEPTOR BONDS IN $Na^+ Fe_{18}$ ← $[SM3]^-$

The charge of a particular iron atom	Name of bonds with heteroatom	quantum chemically calculated length relationships, A	The charge of a particular iron atom	Name of bonds with heteroatom	quantum chemically calculated length relationships, A
−0.368	$Fe–_2C$ $Fe–_1N$	2.36 2.26	−0.394	$Fe–_6O$ $Fe–CH_3$	2.29 2.36
−0.347	$Fe–_4C$ $Fe–_7O$	2.42 2.18	−0.273	$Fe–_8N$ $Fe–CH_3$	2.38 2.44
−0.372	$Fe–_8N$	2.20	−0.299	$Fe–_7O$ $Fe–_6O$	2.23 2.43
−0.222	$Fe–_8N$ $Fe–_9O$	2.38 2.26	−0.352	$Fe–_4C$ $Fe–_7O$	2.46 2.30
−0.248	$Fe–_9O$	2.21	−0.338	$Fe–_3C$ $Fe–_6O$	2.43 2.18
−0.300	$Fe–_9O$	2.31	−0.322	$Fe–_1N$ $Fe–_5C$	2.40 2.44
−0.259	$Fe–_5C$	2.44	−0.143	$Fe–_1N$	2.44
−0.368	$Fe–_8N$ $Fe–_2C$	2.26 2.36	−0.551	Fe–A	2.35
−0.200	$Fe–CH_3$	2.40	−0.595	Fe–A	2.40

In $Na^+ Fe_{18}$ ← $[SM3]^-$ there is an anionic center at $_8N$, whose value due to the lack of so complete delocalization (as in the Fe_{20} ← $[SM 7]^-$ anion) is practically reduced to a maximum. At the same time, the charge density at the jelly–atom is practically equal to that in Fe_{10} ← [SM1], since the electro–sorption properties are minimized. The greatest contribution to the inhibition of corrosion is made by $_8N$, $_6O$, and also by the carbon atoms of the benzene ring, probably due to activation of the benzene ring **A** by an electron pair in $_1N$, since the anionic center saturates the sulfonic group with electrons, and the mesomeric effect becomes weaker. The dentateness of SM 3, as a ligand, along nitrogen atoms is equal to VII (IV units account for the anion center). The dentateness of SM 3, as a ligand, for oxygen atoms is equal to IX (VI units account for 2 hydroxy groups, and III for ketogroups). The methyl group shows dentation equal to II.

Table 6.

LENGTHS OF DONOR–ACCEPTOR BONDS IN Fe$_{19}$ ← [SM4]

The charge of a particular atom of iron	Name bonds with heteroatom	quantum chemically calculated length relationships, A	The charge of a particular atom of iron	Name bonds with heteroatom	quantum chemically calculated length relationships, A
−0.498	Fe–$_2$C Fe–$_1$N Fe–$_5$C	2,50 2,24 2,50	−0.393	Fe–$_6$O Fe–$_7$O	2,36 2,37
−0.367	Fe–$_{21}$O Fe–$_{16}$O	2.31 2,45	−0,614	Fe–$_{22}$O Fe–$_{16}$O	2.50 2,43
−0.553	Fe–$_1$N Fe–$_{16}$O Fe–$_{22}$O	2,25 2,49 2,28	−0.423	Fe–$_5$C	2.47
−0.498	Fe–$_4$C Fe–$_7$O Fe–$_8$N	2,50 2,38 2,33	−0.377	Fe–$_4$C Fe–$_7$O	2.45 2.24
−0.526	Fe–$_7$O	2,33	−0.622	Fe–A	2.27
−0.399	Fe–$_3$C Fe–$_6$O	2,32 2,29	−0.563	Fe–A	2.41
−0.301	Fe–$_8$N Fe–$_{14}$C	2,40 2.38	−0.530	Fe–B	1,93
−0.392	Fe–$_6$O Fe–$_8$N Fe–$_{12}$C	2,30 2.46 2.43	−0.526	Fe–B	2,14
−0.173	Fe–$_{21}$O Fe–$_{16}$O	2.42 2.40	−0.614	Fe–C	2,29
−0.264	Fe–$_{13}$C	2,36	−0.579	Fe–C	2,38
−0.563	Fe–$_{16}$O	2,43			

In Fe$_{19}$ ← [SM4], the oxygen atoms of ketogroup and sulphoxyl groups make the greatest contribution to the inhibition of corrosion. The dentinity of SM 4 as a ligand over nitrogen atoms is V (from this there is III to $_8$N, and there is II to $_1$N). Carbon atoms both $_5$C and $_4$C also contribute to inhibition of corrosion. According to the oxygen atoms $_{16}$O and $_{22}$O, the total dentacy is VI, oxygen atoms $_6$O (is III) and $_7$O (is IV) total dentacy is VII, also the inequality of charges on these oxygen atoms is obvious. In connection with the above facts, it is in this investigated molecule that the highest charge density, which occurs on the iron atom (and the strongest inhibition of corrosion), is manifested. **C** cycle exists only in SM 4 and the comparison of donor properties will remain unexplained in this scientific article.

Table 7.

LENGTHS OF DONOR–ACCEPTOR BONDS IN $Na^+ Fe_{20} \leftarrow [SM5]^-$

The charge of a particular atom of iron	*Name bonds with heteroatom*	*quantum chemically calculated length relationships, A*	*The charge of a particular atom of iron*	*Name bonds with heteroatom*	*quantum chemically calculated length relationships, A*
−0.400	Fe–$_2$C Fe–$_1$N	2.36 2.23	−0.307	Fe–CH_3	2.38
−0.291	Fe–$_5$C	2.41	−0.428	Fe–$_{12}$C Fe–$_{13}$C	2.50 2.46
−0.369	Fe–$_5$C Fe–$_1$N	2.45 2.26	−0.225	Fe–CH_3	2,43
−0.378	Fe–$_6$O Fe–$_7$O	2.38 2.38	−0.450	Fe–CH_3 Fe–$_{11}$C	2.40 2.41
−0.420	Fe–$_6$O Fe–$_8$N	2.43 2.40	−0.403	Fe–$_3$C Fe–$_8$N	2.48 2.19
−0.405	Fe–$_6$O Fe–$_7$O	2.48 2.32	−0.525	Fe–$_7$O Fe–$_8$N	2.35 2.23
−0.216	Fe–$_7$O	2.33	−0.568	Fe–A	2.27
−0.607	Fe–$_7$O	2.46	−0.607	Fe–A	2.28
−0.354	Fe–$_6$O Fe–$_4$C	2.36 2.50	−0.483	Fe–B	2.02
−0.205	Fe–$_{14}$C	2.45	−0.530	Fe–B	1.91

In $Na^+ Fe_{20} \leftarrow [SM5]^-$ an anionic center is also present. The greatest contribution to the inhibition of corrosion is made by the atoms $_8$N, $_6$O, $_7$O. Also, the ethyl group serves as the activator of the **B** cycle. In SM 4 and SM 5, it enters the overall mesomeric effect of the molecule, so the carbon atoms of the **B** cycle of SM 5 also participate in the corrosion inhibition mission (increasing the length of the hydrocarbon chain can be very useful). The dentality of SM 5 as a ligand over the oxygen atom is IX (V of them is $_7$O), nitrogen is V (of which III is an anionic center), methyl radical is III. The saturation and alignment of charges on the $_6$O and $_7$O atoms is due to the electrons of the anionic center, i.e. degree of its expression is less than in SM 3, since in SM 5 the distribution of charges on the $_6$O and $_7$O atoms is the same. Unlike SM 4, in SM 5, though the cycle **B** and enters the conjugation chain, but the ethyl radical does not give the charges to distribute evenly.

Conclusion

Application of article approach, such as lack of hydration molecules, the use of pure iron atoms cluster instead of steel, neglect of participation in the adsorption of molecular hydrogen sulphide and its ions, semi–empirical methods of calculation sand 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. Including the correlation method used in [19] and earlier (with respect to sulfonamides) in [22]. 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 ironcomplexes is not seen as superficial, and as an independent organic compound (or rather, the adduct) with well–defined chemical composition, is similar to π–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 [9], not a screening method [14, 15, 20].

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.

Competing interests

The author declares that they have no competing interests.

References:

1. Anusuya, N., Sounthari, P., Saranya, J., Parameswari, K., & Chitra, S. (2015). Quantum chemical study on the corrosion inhibition property of some heterocyclic azole derivatives. *Orient. J. Chem.,* 31, (3), 1741-1750. doi:10.13005/ojc/310355

2. El-Faham, A., Dahlous, Kh. A., Al Othman, Z. A., & El-Mahdy, G. A. (2016). *sym*-Trisubstituted 1,3,5-Triazine Derivatives as Promising Organic Corrosion Inhibitors for Steel in Acidic Solution. *Molecules,* 21, (4), 436. doi:10.3390/molecules21040436

3. El-Faham, A., Osman, S. M., & El-Mahdy, G. A. (2016). Hydrazino-methoxy-1,3,5-triazine Derivatives’ Excellent Corrosion Organic Inhibitors of Steel in Acidic Chloride Solution. *Molecules,* 21, (6), 714. doi:10.3390/molecules21060714

4. Yüce, A. O., Telli, E., Mert, B. D., Kardaş, G., & Yazıcı, B. (2016). Experimental and quantum chemical studies on corrosion inhibition effect of 5,5 diphenyl 2-thiohydantoin on mild steel in HCl solution. *Journal of Molecular Liquids,* 218, 384-392. doi:10.1016/j.molliq.2016.02.087

5. Thirumalairaj, B., & Jaganathan, M. (2016). Corrosion protection of mild steel by a new binary inhibitor system in hydrochloric acid solution. *Egyptian Journal of Petroleum,* 25, (3), 423-432. doi:10.1016/j.ejpe.2015.09.002

6. Verma, Ch., & Quraishi, M. A. (2017). Adsorption behavior of 8,9-bis(4 (dimethyl amino)phenyl)benzo[4,5]imidazo[1,2-a]pyridine-6,7-dicarbonitrile on mild steel surface in 1 M HCl. *Journal of the Association of Arab Universities for Basic and Applied Sciences*, 22, 55-61. Doi:10.1016/j.jaubas.2016.01.003

7. Karthik, G., & Sundaravadivelu, M. (2016). Studies on the inhibition of mild steel corrosion in hydrochloric acid solution by atenolol drug. *Egyptian Journal of Petroleum,* 25, (2), 183-191. doi:10.1016/j.ejpe.2015.04.003

8. Gece, G. (2008). The use of quantum chemical methods in corrosion inhibitor studies. *Corrosion Science,* 50, (11), 2981-2992. doi:10.1016/j.corsci.2008.08.043

9. El-Lateef, H. M. A., Abo-Riya, M. A., & Tantawy, A. H. (2016). Empirical and quantum chemical studies on the corrosion inhibition performance of some novel synthesized cationic gemini surfactants on carbon steel pipelines in acid pickling processes. *Corrosion Science,* 108, 94-110. doi:10.1016/j.corsci.2016.03.004

10. Kalaiarasi, N., & Manivarman, S. (2017). Synthesis, Spectroscopic Characterization, Computational Exploration of 6-(2-(2,4-Dinitrophenylhydrazano)-Tetrahydro-2-Thioxopyrimidin-4(1h)-one. *Orient. J. Chem.,* 33, (1). doi:10.13005/ojc/330136

11. Lee, H.-S., Ryu, H.-S., Park, W.-J., & Ismail, M. A. (2015). Comparative Study on Corrosion Protection of Reinforcing Steel by Using Amino Alcohol and Lithium Nitrite Inhibitors. *Materials,* 8, 251-269. doi:10.3390/ma8010251

12. El Azzouzi, M., Aouniti, A., Tighadouin, S., Elmsellem, H., Radi, S., Hammouti, B., El Assyry, A., Bentiss, F., & Zarrouk, A. (2016). Some hydrazine derivatives as corrosion inhibitors

for mild steel in 1.0 M HCl: Weight loss, electrochemichal, SEM and theoretical studies. *Journal of Molecular Liquids*, 221, 633-641. doi:10.1016/j.molliq.2016.06.0073

13. El-Belghiti, M., Karzazi, Y., Dafali, A., Hammouti, B., Bentiss, F., Obot, I. B., Bahadur, I., & Ebenso, E. E. (2016). Experimental, quantum chemical and Monte Carlo simulation studies of 3,5-disubstituted-4-amino-1,2,4-triazoles as corrosion inhibitors on mild steel in acidic medium. *Journal of Molecular Liquids*, 218, 281-293. doi:10.1016/j.molliq.2016.01.076

14. Özcan, M., Dehri, I., & Erbil, M. (2004). Organic sulphur-containing compounds as corrosion inhibitors for mild steel in acidic media: correlation between inhibition efficiency and chemical structure. *Applied Surface Science*, 236, (1), 155-164

15. Scendo, M., & Uznanska, J. (2011). Inhibition Effect of 1-Butyl-4-Methylpyridinium Tetrafluoroborate on the Corrosion of Copper in Phosphate Solutions. *International Journal of Corrosion, 2011, 789-801*. doi:10.1155/2011/761418

16. Parr, R. G., & Pearson, R. G. (1983). Absolute hardness: companion parameter to absolute electronegativity. *J. Am. Chem. Soc.*, 105, 7512-7516

17. Parr, R. G., Szentpaly, L., & Liu, S. (1999). Electrophilicity Index. *J. Am. Chem. Soc.*, 121, 1922-1930

18. Pearson, R. G. (2005). Chemical hardness and density functional theory. *J. Chem. Ski*, 117, (5), 369-377

19. Ramkumar, S, & Nalini, D. (2015). Correlation between inhibition efficiency and chemical structure of new indolo imidazoline on the corrosion of mild steel in molar HCl with DFT evidences. *Orient. J. Chem.*, 31, (2), 1057-1064. doi:10.13005/ojc/310255

20. Gonzalez-Olvera, R., Roman-Rodriguez, V., Negron-Silva 1, G. E., Espinoza-Vazquez, A., Rodriguez-Gomez, F. J., Santillan R. (2016). Multicomponent Synthesis and Evaluation of New 1,2,3-Triazole Derivatives of Dihydropyrimidinones as Acidic Corrosion Inhibitors for Steel. *Molecules*, 21, (2), 250. doi:10.3390/molecules21020250

21. Sasikala, T., Parameswari, K., & Chitra, S. (2016). Synthesis and Corrosion Inhibition Study of Benzothiazepine Derivatives on Mild Steel in Acid Medium. *Orient. J. Chem.*, 32, (2). doi:10.13005/ojc/320248

22. Kolesnikova, N. V. (2004). Vliyanie proizvodnykh sulfanilamidov i ureidov na elektroosazhdenie splava Ni-Mn, ego korroziyu v prisutstvii sulfatredutsiruyushchikh bakterii i mitselialnykh gribov i absorbtsiyu vodoroda: avtoref. dis. … kand. khim. nauk. Kaliningrad, 17

23. Reutov, O. A., Kurts, A. L., & Butin, K. P. (2010). Organicheskaya khimiya. Izd. 3-e. Moscow, MGU, Laboratoriya znanii, 1, 700

Список литературы:

1. Anusuya N., Sounthari P., Saranya J., Parameswari K., Chitra S. Quantum chemical study on the corrosion inhibition property of some heterocyclic azole derivatives // Orient. J. Chem. 2015. V. 31. №3. P. 1741-1750. DOI: 10.13005/ojc/310355.

2. El-Faham A., Dahlous Kh. A., AL Othman Z. A., El-Mahdy G. A. sym-Trisubstituted 1,3,5-Triazine Derivatives as Promising Organic Corrosion Inhibitors for Steel in Acidic Solution // Molecules. 2016. V. 21. №4. P. 436. DOI: 10.3390/molecules21040436.

3. El-Faham A., Osman S. M., El-Mahdy G. A. Hydrazino-methoxy-1,3,5-triazine Derivatives' Excellent Corrosion Organic Inhibitors of Steel in Acidic Chloride Solution // Molecules. 2016. V. 21. №6. P. 714. DOI:10.3390/molecules21060714.

4. Yüce A. O., Telli E., Mert B. D., Kardaş G., Yazıcı B. Experimental and quantum chemical studies on corrosion inhibition effect of 5,5 diphenyl 2-thiohydantoin on mild steel in HCl solution // Journal of Molecular Liquids. 2016. V. 218. P. 384-392. DOI: 10.1016/j.molliq.2016.02.087.

5. Thirumalairaj B., Jaganathan M. Corrosion protection of mild steel by a new binary inhibitor system in hydrochloric acid solution // Egyptian Journal of Petroleum. 2016. V. 25. №3. P. 423-432. DOI: 10.1016/j.ejpe.2015.09.002.

6. Verma Ch., Quraishi M. A. Adsorption behavior of 8,9-bis(4 (dimethyl amino)phenyl)benzo[4,5]imidazo[1,2-a]pyridine-6,7-dicarbonitrile on mild steel surface in 1 M HCl // Journal of the Association of Arab Universities for Basic and Applied Sciences. 2017. V. 22. P. 55-61. DOI: 10.1016/j.jaubas.2016.01.003.

7. Karthik G., Sundaravadivelu M. Studies on the inhibition of mild steel corrosion in hydrochloric acid solution by atenolol drug // Egyptian Journal of Petroleum. 2016. V. 25. №2. P. 183-191. DOI: 10.1016/j.ejpe.2015.04.003.

8. Gece G. The use of quantum chemical methods in corrosion inhibitor studies // Corrosion Science. 2008. V.50. №11. P. 2981-2992. DOI: 10.1016/j.corsci.2008.08.043.

9. El-Lateef H. M. A., Abo-Riya M. A., Tantawy A. H. Empirical and quantum chemical studies on the corrosion inhibition performance of some novel synthesized cationic gemini surfactants on carbon steel pipelines in acid pickling processes // Corrosion Science. 2016. V. 108. P. 94-110. DOI: 10.1016/j.corsci.2016.03.004.

10. Kalaiarasi N., Manivarman S. Synthesis, Spectroscopic Characterization, Computational Exploration of 6-(2-(2, 4-Dinitrophenylhydrazano)-Tetrahydro-2-Thioxopyrimidin-4(1h)-one // Orient. J. Chem. 2017. V. 33. №1. DOI : 10.13005/ojc/330136.

11. Lee H.-S., Ryu H.-S., Park W.-J., Ismail M. A. Comparative Study on Corrosion Protection of Reinforcing Steel by Using Amino Alcohol and Lithium Nitrite Inhibitors // Materials 2015. №8. P. 251-269. DOI: 10.3390/ma8010251.

12. El Azzouzi M., Aouniti A., Tighadouin S., Elmsellem H., Radi S., Hammouti B., El Assyry A., Bentiss F., Zarrouk A. Some hydrazine derivatives as corrosion inhibitors for mild steel in 1.0 M HCl: Weight loss, electrochemichal, SEM and theoretical studies // Journal of Molecular Liquids. 2016. V. 221. P. 633-641. DOI: 10.1016/j.molliq.2016.06.0073.

13. El-Belghiti M., Karzazi Y., Dafali A., Hammouti B., Bentiss F., Obot I. B., Bahadur I., Ebenso E. E. Experimental, quantum chemical and Monte Carlo simulation studies of 3,5-disubstituted-4-amino-1,2,4-triazoles as corrosion inhibitors on mild steel in acidic medium // Journal of Molecular Liquids. 2016. V. 218. P. 281-293. DOI: 10.1016/j.molliq.2016.01.076.

14. Özcan M., Dehri I., Erbil M. Organic sulphur-containing compounds as corrosion inhibitors for mild steel in acidic media: correlation between inhibition efficiency and chemical structure // Applied Surface Science. 2004. V. 236. №1. P. 155-164.

15. Scendo M., Uznanska J. Inhibition Effect of 1-Butyl-4-Methylpyridinium Tetrafluoroborate on the Corrosion of Copper in Phosphate Solutions // International Journal of Corrosion. 2011. V. 2011. P. 789-801. DOI: 10.1155/2011/761418.

16. Parr R. G., Pearson R. G. Absolute hardness: companion parameter to absolute electronegativity // J. Am. Chem. Soc. 1983. V. 105. P. 7512-7516.

17. Parr R. G., Szentpaly L., Liu S. Electrophilicity Index // J. Am. Chem. Soc. 1999. V. 121. P. 1922-1930.

18. Pearson R. G. Chemical hardness and density functional theory // J. Chem. Ski. 2005. V. 117. № 5. P. 369-377.

19. Ramkumar S., Nalini D. Correlation between inhibition efficiency and chemical structure of new indolo imidazoline on the corrosion of mild steel in molar HCl with DFT evidences // Orient. J. Chem. 2015. V. 31. №2. P. 1057-1064. DOI: 10.13005/ojc/310255.

20. Gonzalez-Olvera R., Roman-Rodriguez V., Negron-Silva 1 G. E., Espinoza-Vazquez A., Rodriguez-Gomez F. J. Santillan R. Multicomponent Synthesis and Evaluation of New 1,2,3-Triazole Derivatives of Dihydropyrimidinones as Acidic Corrosion Inhibitors for Steel // Molecules. 2016. V. 21. №2. P. 250. DOI: 10.3390/molecules21020250.

21. Sasikala T., Parameswari K., Chitra S. Synthesis and Corrosion Inhibition Study of Benzothiazepine Derivatives on Mild Steel in Acid Medium // Orient. J. Chem. 2016. V. 32. №2. P. 1215-1222. DOI: 10.13005/ojc/320248.

22. Колесникова Н. В. Влияние производных сульфаниламидов и уреидов на электроосаждение сплава Ni-Mn, его коррозию в присутствии сульфатредуцирующих бактерий и мицелиальных грибов и абсорбцию водорода: автореф. дис. … канд. хим. наук. Калининград, 2004. 17 с.

23. Реутов О. А., Курц А. Л., Бутин К. П. Органическая химия. Изд. 3-е. М: МГУ, Лаборатория знаний, 2010. Т. 1. 700 с.

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