Chemical Methodologies

Original Research article

Polyaminopolyphosphonates and Polyaminopolycarbonoates (that are "Chelators") in Mission of Inhibiting of Microbiological Corrosion with Desulfovibrio Desulfuricans

Sikachina Andrey Anatolevich[a] *, Beloglazov Sergey Michailovich[b]

[a] Chemical and Biological Institute, Immanuel Kant Baltic Federal University, Kaliningrad-City, Russian Federation. SPIN-code: 8133-3363
[b] Chemical and Biological Institute, Immanuel Kant Baltic Federal University, Kaliningrad-City, Russian Federation

ARTICLE INFORMATION

ABSTRACT

In this paper, the process of adsorption of organic compounds of the polyaminopolyphosphonates and polyaminopolycarbonoates (chelators or complexones) chemical type on iron (available in steel St3S (Poland) 97%) is modeled using the HyperChem package version 8.0.7 with semi-empirical ZINDO / 1 method. The structures of chelators ("complexones") 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.

Corresponding author: E-mail: sikachina@list.ru
Immanuel Kant Baltic Federal University, Kaliningrad-City, Russian Federation. Tel:+79520559717

Graphical Abstract
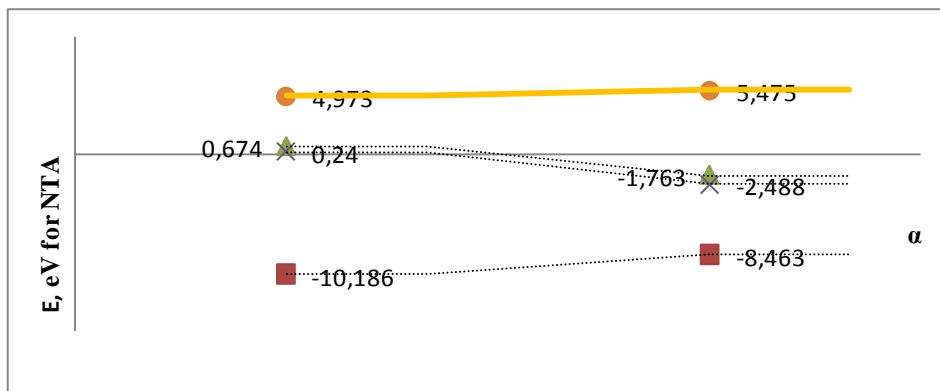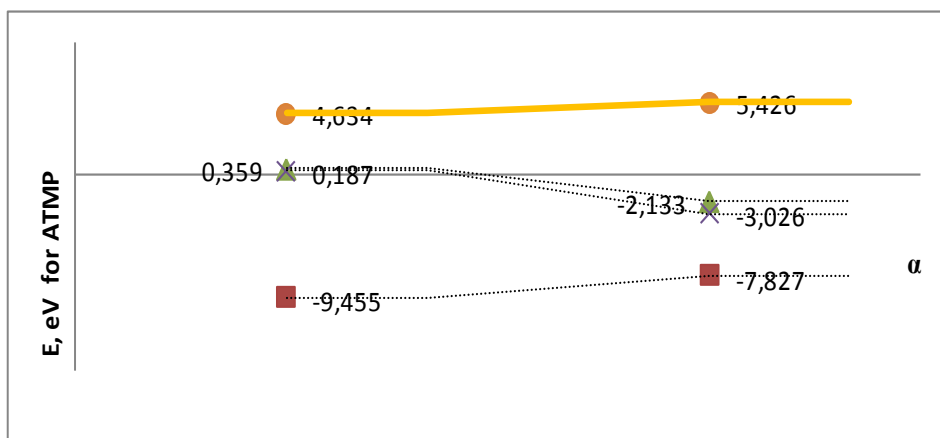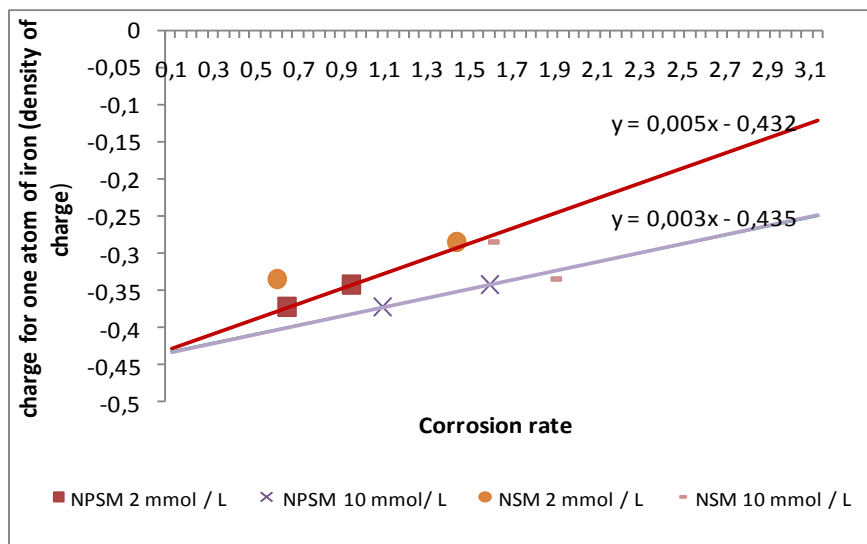
List of accepted abbreviations by author:

SRB - sulfate-reducing bacteria

K - corrosion rate

SM - the studied molecule

NP SM - researched molecule of polyaminopolyphosphonates

N SM - researched molecule of polyaminopolycarbonoates

N (ac): N (d) - ratio indicating balance between the amount of donor and acceptor groups of the molecules

$FF_{\Delta\eta}$ - Fukui function, calculated from molecular rigidity

O^h - oxygen atom of the hydroxy

O^k - keto oxygen atom

$O^{h/f}$- oxygen/phosphoryl group

Σq is a value of the total charge, is given by: $\Sigma q = {_1}q + {_2}q$

Δq is changing the amount of charge in the formation of a complex of iron chelator molecule

HOMO - the highest filled molecular orbital

LUMO - the lowest free molecular orbital

1 LUMO - orbital, the next lowest free molecular orbital

ω - the value of the global electrophilicity

$\omega\Sigma q$ is the magnitude of the local electrophilicity particular atom

$_{Fe}\rho_q$ is the charge for one atom of iron (density of charge)

Introduction

The current state of evidence on polyaminopolyphosphonates and polyaminopolycarbonoates (complexone or chelators or SM) as the corrosion inhibitors is very average. In general, the compounds of this class have been studied as inhibitors of ordinary electrochemical corrosion in cooling systems [8], hot water systems [6], refining [18] for the purification of metals and alloys against corrosion films [4], in concentrated brines [2], and the influence of the cations and anions on manifestation of the inhibitory effect [17, 19]. Extensive studies have been conducted only for some members of chelators such as HEMPA, ATMP, EDTA.

Scientists at the Institute of Physical and Colloid Chemistry (IPCC of RAoS, Moscow, Russia), the protective effect of Zn^{2+}-HEMPA explained by the formation of mixed poorly soluble complex compounds of Zn^{2+} and Fe^{3+} with HEMPA and partial deposition $Zn(OH)_2$ on the metal surface. Zn^{2+}-HEMPA is an inhibitor of the mixed action, braking, mainly cathodic process, the kinetics of which

are very little affected by the presence of CI^- [13]. The high efficiency of Zn^{2+}-HEMPA mission in inhibiting corrosion in aqueous solutions, and also aluminum and other non-ferrous alloys [6, 8, 13].

However, not too many microbiological corrosion studies were conducted [5, 8]. Verity of studies have been conducted in the Tambov State University and Baltic Federal University (Russia). Corrosion of different metals in aggressive acidic, for example, [1, 3, 7, 12, 14, 15, 16] and salt [24] medium are investigated a very large number of scientists worldwide.

Many of the organic compounds that perform the mission of protecting corrosion [1, 7, 16], have been investigated by the approach "structure-property" using the Pearson correlation coefficient, for example, [1, 5, 21, 11]. Chelators as inhibitors of microbial corrosion SRB-creator of content were first investigated [22]. In addition, the author was modeled adsorption process on iron of chelators; iron is part of steel. Simulation reactivity of organic compounds was undertaken in the past [10], in particular, the simulation of adsorption on the metal clusters of organic compounds described hypothetical cluster where the metal surface [25, 26]. Contributed by the author changes in cluster modeling method suggest it is an organic compound adsorption capabilities with regard, in particular, to iron, and therefore there is a new value of the "charge density on the iron", i.e. the proportion of the electron density which passed from the organic compound converted for an individual iron atom [23].

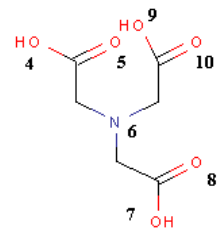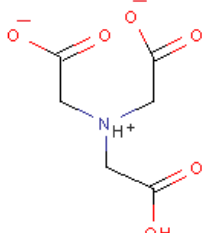## Experimental

Material and Methods
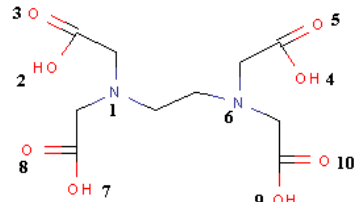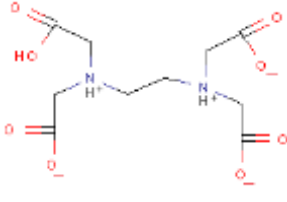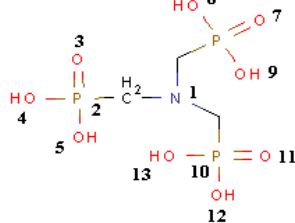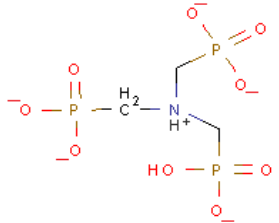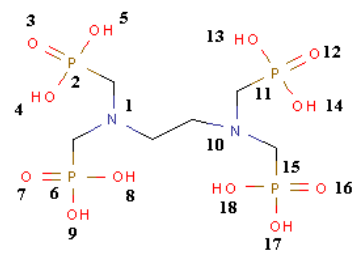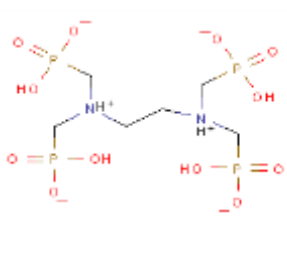
A variety of microbiological corrosion system

In the article investigated the heterogeneous thermodynamic system of closed type "St3S/breeding ground of Postgate of "B" class + *Desulfovibrio desulfuricans* cells" [5], samples of steel were parameters 20×50×1 mm and Samples of steel were taken from one batch which guaranteed them the same chemical composition [11].

Organic compounds - corrosion inhibitors

This study which employed SM manifests an ability to inhibit microbiological corrosion highly dependent not only on the structure of the molecule, but also on the pH [22]. In such transitions, the electron density in the SM is not introduced or removed, and quantum chemical calculations and estimates based on them were taken classical formulas, almost perfectly describes a pH-dependent structure of the SM (Table 1).

Table 1. Test compounds and adopted (by author) numbering significant heteroatoms

Abbreviation of inhibitor	Classic structural formula	pH-dependent structural formula
NTA		
EDTA		
ATMP		
EDTMP		

The validity of adopting classical formula

The validity of the adoption of classical formulas of complex ones as an onium-type SM has been confirmed by means of quantum-chemical calculations previously performed by the author of the descriptors of the electronic structure of the forms of molecules of these SMs.

Table 2. The calculated values of the conversion factors for the conversion of the most likely forms of molecules of complexones into classical forms (calculated by quantum-chemical methods (DFT/B3-LYP/3-21G *))

Abbreviation of inhibitor	The values of the transfer coefficients *k*, equal to $\Sigma_{pH}descriptor_{sm} : \Sigma_{clas}descriptor_{sm}$, for example				
	$k(\Delta E)$	$k(\sum Q_N)$	$k(\sum Q_P)$	$k(\sum Q_o^h)$	$k(\sum Q_o^{f/k})$
EDTMP	0,679	1,088	0,971	0,950	1,089
ATMP	0,646	1.089	0,970	0.993	1.060
EDTA	0,570	1,120	-	0,959	1,004
NTA	0,555	1,025	-	0,995	1.113

It was found that the *pH-dependent* forms of SM molecules are smaller by approximately 2 times (in N SM) and 1.5 times (in NP SM) values of energy gaps, and also the fact that the charges on heteroatoms of such forms of molecules are practically equal charges taking place in the classical structure. Moreover, each of the coefficients, tied to the same descriptor of all SMs, is stable or more or less than one, which proves the identical distribution of descriptors of the classical structure and pH-dependent form of complexones.

The protective effect against corrosion

Data on corrosion rates obtained by the standard method of gravimetric analysis [5] were taken from [22]. According to [21], the above structure was a structural series of molecules.

The technology of quantum chemical calculations

The calculation was performed using HyperChem 8.0.7. Software, empirically, the limit was set by the number of iron atoms: a number *a*, when out of *(a+b)* given by HyperChem-user iron atoms carrying zero charge number *b*. The plane of neutral iron atoms specified by the user of HyperChem was 1, 2. 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. Then, it was assumed that the SM donor possibilities are exhausted. Equation electrophilic reaction is *a* Fe⁰+SM Y=[SMY]→Fe*a*, in which iron atoms are acceptors being charged

negatively. Finding the values of quantum chemical descriptors held level theory OPLS/PM3/ ZINDO/1. [9, 11, 23]. Mesomeric effect was taken into account, which is manifested in different parts of the investigated SM. In the following controlled descriptors of electronic structure: charges on heteroatoms (by Mulliken) will be calculated as Σq, i.e. charges on the same arrangement of atoms will be summarized as a result of a high degree of symmetry of the test running, the energy frontier orbitals, the resulting composition [SMY] → Fe$_a$, in which the SM acts as a ligand. Based on these characteristics will be calculated from the data file. *out*: the charge density on the iron (1 atom of Fe), global and local electrophilicity, consider the complex structure. Along the length of bond «Fe-*heteroatom*" taken into account within the 3.00 angstroms (A).

The above simulation technology has been developed by the author for the first time tested on a number of organic compounds in Russia in 2015.

Results and discussion

The generated quantum chemically molecular parameters shown diagram, made in the form specified in [20] in Scheme 1-4:
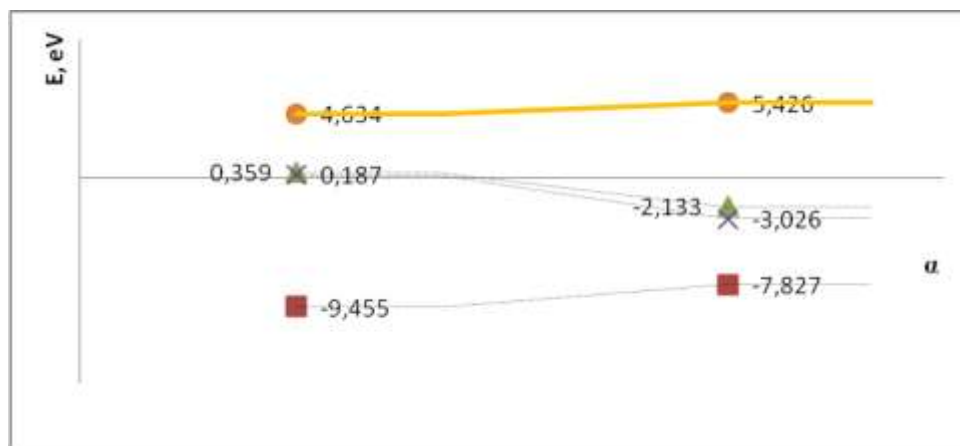
Scheme 1. The energy levels of HOMO (■), LUMO (✕), 1LUMO(▲), and the positions of the molecules hardness (●) in the formation of the adsorption complex (right) with ATMP (left)
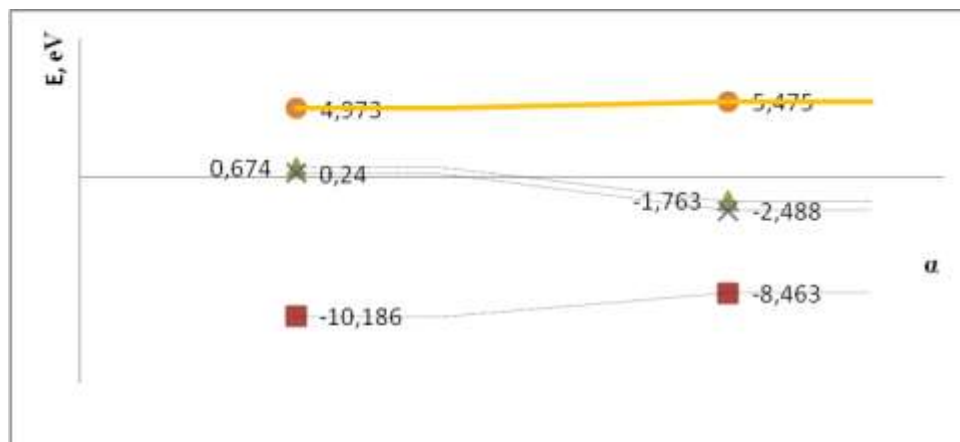
Scheme 2. The energy levels of HOMO (■), LUMO (✕), 1LUMO(▲), and the positions of the molecules hardness (●) in the formation of the adsorption complex (right) with NTA (left)
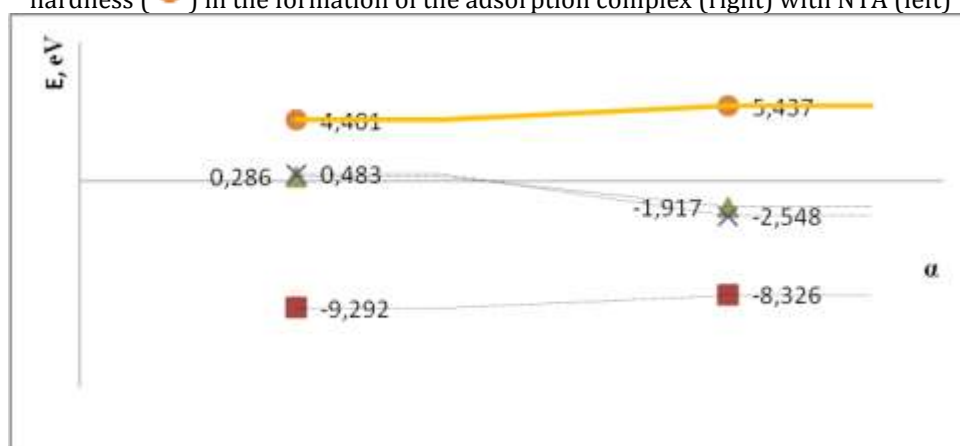
Scheme 3. The energy levels of HOMO (■), LUMO (✕), 1LUMO(▲), and the positions of the molecules hardness (●) in the formation of the adsorption complex (right) with EDTMP (left)
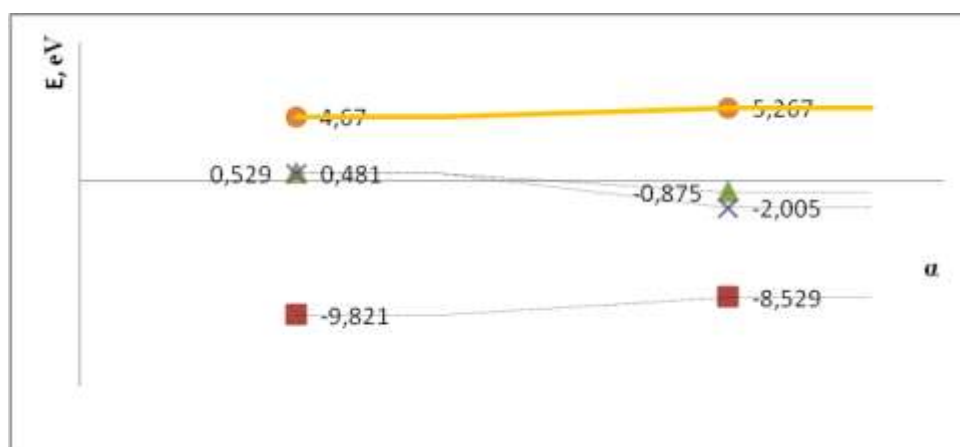
Scheme 4. The energy levels of orbitals HOMO (■), LUMO (✕), 1LUMO(▲), and the positions of the molecules hardness (●) in the formation of the adsorption complex (right) with EDTA (left)

The isolated molecules are nucleophilic. As ligands are electrophiles, the rigidity of the ligand molecule, (especially NP SM class) after adsorption, increases, so [SMY] → Fe_a can be nonpolarizable that confirms the ability to inhibit microbial corrosion. Obviously, the charts give the impression of the same mechanism ironcomplexones generation, so it can be assumed that the criterion of uniform symmetrical complexity of the structure does not affect the adsorption process [23]. In all cases the HOMO increases from baseline SM, LUMO and 1LUMO, the value of the stiffness of the molecule-increases similar to the HOMO. Effective charges (by Mulliken) on parts of the SMY are shown in Table 3.

Table 3. Illustration of the charge changes in different states complexones

| Abbreviations of chelators	$\sum_h \Delta q_O$	$\sum_{f/k} \Delta q_O$	$\sum \Delta q_N$	$\sum \Delta q_P$
charge distribution in the starting molecules				
ATMP	-4,139	-2,649	0,023	6,311
NTA	-0,864	-1,157	-0,042	—
EDTMP	-5,520	-3,573	-0,046	8,392
EDTA	-1,213	-1,552	-0,108	—
charges distribution in the ligands - the final states of the original molecules				
ATMP	-0,916	-0,313	-0,033	2,276
NTA	-0,288	-0,170	0,041	—
EDTMP	-1,101	-0,380	0,024	3,166
EDTA	-0,522	-0,237	0,015	—

The distribution is quite common, as is happening with heteroatom Donation of electron density at the iron atoms (positive charges are sharply). Obviously, the keto oxygen atoms and electrons are depleted phosphoryl ("centers of adsorption"), the rest of the atoms investigated structures the charge density is substantially reduced down to zero (nitrogen and phosphorus, as "adsorption sites"). Least of all is expressed in EDTMP, because it has a large number of negative charges. Donation takes place both at the expense of the native electron density, and due to its overflow from the other groups. The values of ω and $_{Fe}\rho_q$ of NP SM are shown in Table 4.

Table 4. The values of electrophilicity, the charge density for atom of iron compounds formed ironcomplexones of NP SM

Abbreviations of chelators	$_{Fe}\rho_q$	ω	The compositions of the complex compounds, a
ATMP	-0,342	1,113	14
NTA	-0,285	1,185	14
EDTMP	-0,372	0,992	20
EDTA	-0,335	1,059	19

Values of local electrophilicity of heteroatoms with N SM, values of [N (a): N (d)], values of $(FF_{\Delta\eta})$ are shown in Table 5.

Table 5. The values of the local electrophility of heteroatom. Values in parentheses are the translation of the local electrophility for 1 atom or group for fair comparisons

Abbreviations of complexones	$\omega\sum q_N(\omega q_N)$	$\omega\sum_h q_O$ $(\omega_h q_O)$	$\omega\sum q_P\ (\omega q_P)$	[N (ac):N (d)]/[(FF$_{\Delta\eta}$)]	$\omega\sum_{f/\kappa} q_O$ $(\omega_{f/\kappa} q_O)$
ATMP	-0,062 (-0,062)	3,591 (0,598)	-4,492 (-1,497)	[3]/[-2.44]	2,601 (0,867)
NTA	0,098 (0,098)	0,659 (0,220)	—	[3] /[-2.23]	1,171 (0,390)
EDTMP	0,069 (0,034)	4,332 (0,541)	-5,182 (-1,295)	[2]/ [-1.98]	3,175 (0,794)
EDTA	0,129 (0,064)	0,731 (0,183)	—	[2]/[-1,89]	1,392 (0,348)

In N SM *a* is more than N SM, because the former has lower power and chemisorption centers. There is a direct correlation between the composition ironcomplexones NP SM and N SM and value SM Y ligand. ω of the N SM is the greatest at the NTA, and of NP SM from ATMP. In general, the donor properties (which are the higher, the lower the local electrophilicity), which are fundamental to the mission of inhibitor of corrosion protection, are inversely proportional to the value of [N (ac): N (d)] and, apparently, as a consequence, the value of $(FF_{\Delta\eta})$. It should be noted that the activity of the donor of the phosphoryl oxygen atoms (in NP SM) most low in ATMP, may be associated with steric hindrance. This version is confirmed by comparing the N SM, where donor activity of ketogroups on the basis of a comparison of the corresponding local electrophilic also quite similar, but the steric hindrance present here, but judging by the structural formula of NTA, they should appear less intense as obvious as NTA less donor is active, than EDTA. Special mention should be on the phosphorus atoms. They strongly nucleophilic, that may be associated to the decrease in the electronegativity greater and their valency and on them is that the outflow from the electron density of the iron atoms of the iron atoms in the nucleus therefore more strongly attracted to the phosphorus atoms. $\omega\sum\Delta q_P$ The value is negative, that may be associated to, first, the traditionally higher charges on the atoms in the interpretation of semi-empirical methods, and secondly, to the phosphorus atom chemisorption on a negatively charged metal surface, causing it becoming part of the electron density of the surface. This phenomenon contributes to the increase in the charge density on the iron atom, and also confirms the view of the possibility of moving electrosorption in

chemisorption. $\omega\sum_f\Delta q_0$ can also be associated to the value of the molar mass of the test compound. For all cases examined, it was revealed that the iron atoms, in general, belong to a particular molecule under consideration, and largely localized forces donor-acceptor interaction in some parts of the molecule. For NTA ironcomplexone following structure (Table 6).

Table 6. Characteristics of bonds in the $Fe_{14}NTA$

The charge of a particular atom of iron	Name of bonds with heteroatom	quantum chemically calculated length of relationships, A	The charge of a particular atom of iron	Name of bonds with heteroatom	quantum chemically calculated length of relationships, A
-0,478	$Fe_{-9}O^h$ Fe-N $Fe_{-7}O^h$	2,30 2,23 2,33	-0,219	$Fe_{-7}O^h$ $Fe_{-8}O^к$	2,65 2,21
-0,175	$Fe_{-4}O^h$ $Fe_{-3}O^к$	2,65 2,38	-0,426	$Fe_{-10}O^к$ $Fe_{-7}O^h$ $Fe_{-8}O^к$	2,51 2,68 2,42
-0,172	$Fe_{-4}O^h$ $Fe_{-3}O^к$	2,54 2,43	-0,194	$Fe_{-9}O^h$ $Fe_{-10}O^к$	2,78 2,27
-0,231	$Fe_{-3}O^к$	2,41	-0,247	$Fe_{-10}O^к$	2,30
-0,278	$Fe_{-3}O^к$	2,41	-0,198	$Fe_{-9}O^h$ $Fe_{-10}O^к$	2,41 2,41
-0,253	$Fe_{-7}O^h$	2,43	-0,386	$Fe_{-4}O^h$ Fe-N	2,41 2,33
-0,268	$Fe_{-8}O^к$	2,25	-0,461	$Fe_{-4}O^h$ $Fe_{-9}O^h$ Fe-N	2,37 2,39 2,76

The structure of both NTA are obvious in which Fe atoms, with respect to the coordination number of heteroatom atoms, are within the range of I ... III. In many cases, the higher the charge on the iron atom, the coordination number higher value. The highest coordination numbers are observed in the iron atoms with $Q(Fe) \geq -0.4$. The shortest bondes are $Fe-O^к$ and Fe-N (about 2.2 ... 2.4 A), the longest bond is $Fe-O^h$ (about 2,5 ... 2,7A). Denticity of hydroxyl oxygen atoms are equal to IV, denticity of by oxygen atoms keto III ... IV. Denticity on the nitrogen atom is III. For ATMP ironcomplexone following structure (Table 7).

Table 7. Characteristics of bonds in the Fe_{14} ATMP

The charge of a particular atom of iron	Name bonds to heteroatom atoms	quantum chemically calculated length relationships, A	The charge of a particular atom of iron	Name bonds to heteroatom atoms	quantum chemically calculated length relationships, A
-0,229	$Fe\text{-}_3O^f$ $Fe\text{-}_2P$ $Fe\text{-}_4O^h$	2,38 2,82 2,36	-0,442	$Fe\text{-}_{13}O^h$ $Fe\text{-}_{12}O^h$ $Fe\text{-}_4O^h$ $Fe\text{-}_8O^h$ $Fe\text{-}_7O^f$ $Fe\text{-}_9O^h$ $Fe\text{-}_6P$	2,19 2,93 2,43 2,35 2,71 2,92 2,97
-0,313	$Fe\text{-}_3O^f$ $Fe\text{-}_2P$ $Fe\text{-}_5O^h$	2,44 2,66 2,99	-0,568	$Fe\text{-}N$ $Fe\text{-}_2P$ $Fe\text{-}_3O^f$ $Fe\text{-}_6P$ $Fe\text{-}_7O^f$	2,88 2,73 2,46 2,70 2,36
-0,193	$Fe\text{-}_4O^h$ $Fe\text{-}_5O^h$ $Fe\text{-}_2P$ $Fe\text{-}_{12}O^h$	2,52 2,28 2,97 2,36	-0,276	$Fe\text{-}_8O^h$ $Fe\text{-}_7O^f$	2,47 2,25
-0,547	$Fe\text{-}_5O^h$ $Fe\text{-}_{12}O^h$ $Fe\text{-}_{10}P$ $Fe\text{-}N$ $Fe\text{-}_2P$	2,41 2,36 2,69 2,85 2,74	-0,286	$Fe\text{-}_6P$ $Fe\text{-}_8O^h$	2,79 2,35
-0,366	$Fe\text{-}_{11}O^f$ $Fe\text{-}_{10}P$	2,17 2,69	-0,155	$Fe\text{-}_8O^h$ $Fe\text{-}_6P$ $Fe\text{-}_9O^h$	2,43 2,87 2,26
-0,352	$Fe\text{-}_{11}O^f$ $Fe\text{-}_{12}O^h$ $Fe\text{-}_{10}P$ $Fe\text{-}_{13}O^h$	2,25 2,43 2,64 2,83	-0,518	$Fe\text{-}_6P$ $Fe\text{-}_9O^h$ $Fe\text{-}N$ $Fe\text{-}_{10}P$ $Fe\text{-}_{12}O^h$	2,81 2,36 2,75 2,80 2,25
-0,359	$Fe\text{-}N$	2,23	-0,188	$Fe\text{-}_2P$ $Fe\text{-}_3O^f$ $Fe\text{-}_5O^h$	2,82 2,37 2,59

It is obvious that the iron atoms with respect to the heteroatoms have a coordination number of values in the range II … VII. The highest coordination numbers are observed in the iron atoms with Q (Fe) = -0.4 … -0,5. Proportionality depending on the charge of the iron atom that atom valences exhibited sufficiently clearly observed (e.g., Fe-5 and Fe-6). The shortest bond is $Fe\text{-}O^f$ (about 2.2 … 2.5 A), the longest are $Fe\text{-}O^h$ (about 2.3 … 2.9 A) and Fe-P (about 2.7 … 3.0 A). In general, the longer

the bond, the more pronounced degree of ionicity. Dentate on phosphorus atoms is IV … VI, denticity of hydroxyl oxygen atoms equal III … V, denticity of by oxygen atoms of the phosphoryl group is II … IV. IV is denticity of nitrogen atom. For EDTA ironcomplexone following structure (Table 8).

Table 8. Characteristics of bonds in the $Fe_{19}EDTA$

The charge of a particular atom of iron	Name bonds to heteroatom atoms	quantum chemically calculated length relationships, A	The charge of a particular atom of iron	Name bonds to heteroatom atoms	quantum chemically calculated length relationships, A
-0,254	$Fe-_2O^h$	2,30	-0,331	$Fe-_6N$	2,39
-0,386	$Fe-_3O^к$ $Fe-_8O^к$	2,35 2,18	-0,159	$Fe-_3O^к$	2,29
-0,352	$Fe-_8O^к$	2,35	-0,168	$Fe-_2O^h$ $Fe-_4O^h$	2,41 2,53
-0,302	$Fe-_7O^h$	2,19	-0,420	$Fe-_2O^h$ $Fe-_3O^к$ $Fe-_4O^h$	2,55 2,45 2,44
-0,561	$Fe-_3O^к$ $Fe-_8O^к$ $Fe-_1N$	2,25 2,44 2,24	-0,219	$Fe-_4O^h$ $Fe-_5O^к$	2,73 2,23
-0,468	$Fe-_3O^к$ $Fe-_9O^h$ $Fe-_{10}O^к$ $Fe-_6N$	2,27 2,65 2,57 2,36	-0,423	$Fe-_6N$ $Fe-_5O^к$ $Fe-_{10}O^к$	2,65 2,44 2,35
-0,532	$Fe-_6N$ $Fe-_9O^h$	2,83 2,39	-0,235	$Fe-_4O^h$	2,38
-0,225	$Fe-_{10}O^к$ $Fe-_9O^h$	2,24 2,47	-0,588	$Fe-_6N$ $Fe-_2O^h$ $Fe-_4O^h$	2,90 2,48 2,52
-0,264	$Fe-_9O^h$ $Fe-_{10}O^к$	2,99 2,62	-0,329; -0,152	$Fe-_1N$; $Fe-_9O^h$	2,32; 2.32[1]

There is no clear indicated earlier whichever is the higher charge on the iron atom, the value of the coordination number above. The structure of the EDTA Fe atoms with respect to the coordination number of the heteroatom atoms are within the range of I … IV. The highest coordination numbers are observed in the iron atoms with Q (Fe) = -0,4 … -0,5. It is not possible to identify the shortest

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[1]In this row of the table presents data on the 2 atoms of iron that has been done for reasons of compactness and tables Beauty

bond: as such can be Fe-O^k (about 2.2 … 2.4 A) and Fe-O^h (about 2.2 … 2.5 A), except those of Fe-10 (2.99A) and of Fe-15 (2.7A), the longest - Fe-N (about 2.2 … 2.9 A). Denticity of hydroxyl oxygen atoms is I … V, denticity by ketooxygen atoms is III … V. VII is denticity of nitrogen atoms. This is all explainedto the increasing complexity of simple molecules. For EDTMP iron complex one following structure, (see Table 9).

Table 9. Characteristics of the bonds in the Fe$_{20}$ EDTMP

The charge of a particular atom of iron	Name bonds to heteroatom atoms	quantum chemically calculated length relationships, A	The charge of a particular atom of iron	Name bonds to heteroatom atoms	quantum chemically calculated length relationships, A
-0,276	Fe-$_2$P Fe-$_4$O^h	2,82 2,20	-0,338	Fe-$_{15}$P Fe-$_{16}$O^f	2,70 2,23
-0,314	Fe-$_3$O^f Fe-$_4$O^h	2,17 2,46	-0,474	Fe-$_{18}$O^h Fe-$_{11}$P Fe-$_{14}$O^h Fe-$_{10}$N Fe-$_{15}$P	2,38 2,87 2,43 2,73 2,86
-0,427	Fe-$_1$N Fe-$_7$O^f Fe-$_6$P	2,92 2,28 2,69	-0,377	Fe-$_{10}$N	2,30
-0,309	Fe-$_7$O^f Fe-$_9$O^h Fe-$_6$P	2,18 2,79 2,69	-0,294	Fe-$_{12}$O^f Fe-$_{14}$O^h	2,74 2,31
-0,372	Fe-$_7$O^f Fe-$_6$P Fe-$_8$O^h	2,39 2,69 2,30	-0,141	Fe-$_{14}$O^h Fe-$_{13}$O^h Fe-$_{11}$P	2,27 2,32 2,88
-0,525	Fe-$_3$O^f Fe-$_8$O^h Fe-$_1$N	2,34 2,28 2,21	-0,154	Fe-$_{14}$O^h Fe-$_{17}$O^h	2,29 2,31
-0,268	Fe-$_4$O^h Fe-$_5$O^h Fe-$_2$P	2,20 2,32 2,87	-0,573	Fe-$_{12}$O^f Fe-$_{18}$O^h Fe-$_{13}$O^h Fe-$_{17}$O^h Fe-$_{11}$P Fe-$_{15}$P	2,38 2,74 2,67 2,49 2,71 2,76
-0,611	Fe-$_6$P Fe-$_7$O^h Fe-$_1$N Fe-$_{10}$N Fe-$_{17}$O^h Fe-$_8$O^h	2,74 2,63 2,96 2,98 2,40 2,44	-0,447	Fe-$_{14}$O^h Fe-$_1$N Fe-$_2$P	2.29 2.36 2.91
-0,247	Fe-$_{16}$O^f Fe-$_{15}$P	2,25 2,87	-0.641	Fe-$_3$O^f Fe-$_5$O^h	2.17 2.87

	$Fe\text{-}18O^h$	2,45			$Fe\text{-}12O^f$	2,41
					$Fe\text{-}2P$	2,77
					$Fe\text{-}11P$	2,77
					$Fe\text{-}10N$	2,95
-0,337	$Fe\text{-}18O^h$	2,41	-0,321		$Fe\text{-}11P$	2,74
					$Fe\text{-}12O^f$	2,20
					$Fe\text{-}14O^f$	2,47

In the EDTMP structure, the iron atoms, with respect to the coordination number of heteroatom atoms, are within the range of I ... VI. The highest coordination numbers are observed in the iron atoms with Q (Fe) = -0.5 ... -0,6. The shortest bonds are $Fe\text{-}O^f$ (about 2.2 ... 2.4 A), and Fe-P (on the order of 2.7 ... 2.9 A). Intermediate length can be called $Fe\text{-}O^h$ (about 2.2 ... 2.4 A), except Fe-4 (2.8 A), Fe-17 and Fe-19 (2.9 A), $Fe\text{-}O^h$ (2,6 A). The association with the phosphorus atom is unimportant in the formation of the charge on the iron atom (hence the electron density at the iron in EDTMP slightly higher than that of EDTA). Dentate on the phosphorus atom is II ... V, denticity of hydroxyl oxygen atoms is I ... V, denticity of oxygen atoms of the phosphoryl group is I ... IV. Denticity of nitrogen atoms is VIII.

The dependence of K in the presence of N SM and NP SM on the charge density on the iron expressed is in Scheme 5.
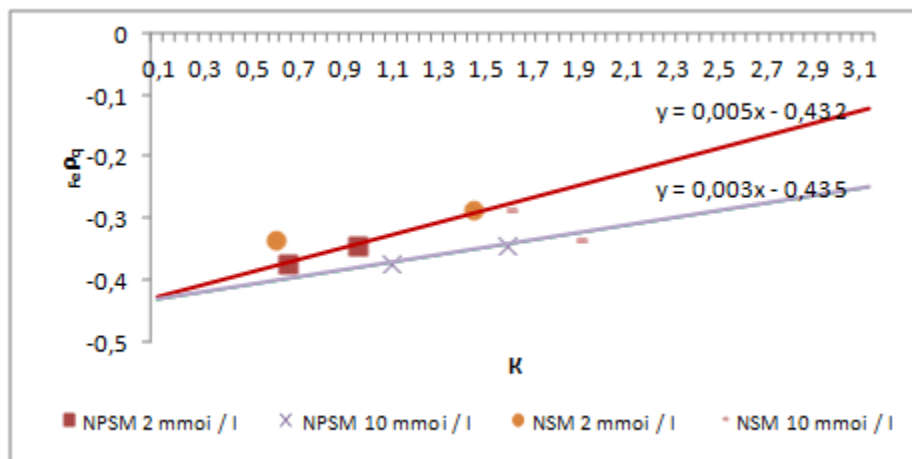
Scheme 5. Dependence of the $_{Fe}\rho_q$-K type

If the graphical dependency were parallel, it would mean that there is no chemisorption component in the effect of inhibiting microbiological corrosion. The greater depth of the outflow of the electron density of the molecule to the iron atoms, the lower K. This pattern is shown using NPSM. Obviously, if this type of corrosion inhibition is caused large bactericidal than adsorption on steel construction and consideration of such dependencies impracticable. For K=0,1, $_{Fe}\rho_q$ is below

0.5, the inhibitory properties lost when $_{Fe}\rho_q$=-0,35 ... -0,30, at a higher density starting promotion of corrosion.

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. 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 are 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, not a screening method.

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.

Obviously, in the case of simple NTA and ATMP, which are formed of the same composition iron complexones molecule, the coordination number of the iron for $Fe_{14}ATMP$ much higher than $Fe_{14}NTA$ - so the first better inhibitor than the second. He also has a higher denticity of nitrogen. Dentate of nitrogen of EDTMP is extremely high and there is a large amount of iron bonds with phosphorus, so this matter will be the best inhibitor. Then will follow the EDTA, the latter - NTA.

Acknowledgement

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