A.H. Mandryka[1], O.O. Pasenko[1], V.H. Vereschak[1], Y.S. Osokin[2]

Modeling of orthosilicate and methanesulfonic acid clusters in aqueous solution

[1]*Ukrainian State University of Chemical Technology, Dnipro, Ukraine*
[2]*Primus Inter Pares School, Dnipro, Ukraine, osokin@cf.dnu.dp.ua*

The possibility of binding orthosilicate acid to different amounts of methanesulfonate anions was considered in this work using quantum chemical modeling. It was demonstrated that methanesulfonic acid forms two hydrogen bonds with an orthosilicate acid molecule, regardless of the conformation of the cluster itself. Based on the results of calculations of the energy parameters of the systems and the boundary molecular orbitals, it was found that the most stable cluster of orthosilicate acid with methanesulfonate anion is $[H_4SiO_4 \cdot 4CH_3SO_3^-]$. It was also found that a characteristic feature of all the studied clusters at the level of electron density distribution is the formation of the eightmembered cycle $(S–O\cdots H–O–Si–O–H\cdots O)$ and $(S–O\cdots H–O–Si–O\cdots H–C)$. The absence of a significant dependence of the effective charge from the silicon atom on the number of methanesulfonate anions in the inner sphere was also found. Thus, it has been theoretically demonstrated that methanesulfonate anion is able to stabilize orthosilicate acid and reduce the possibility of its dimerization.

Keywords: orthosilicate acid; methanesulfonic acid; clusters; aqueous solution; quantum chemical modeling; binding energy; hydrogen bonding.

Introduction

Orthosilicic acid is the main form of silicon(IV) that is soluble in aqueous solution, but it is unstable in this environment [1] and interacts with itself and easily transforms into insoluble polymeric forms [2, 3]. One of the ways to stabilize it in aqueous solution is to bind orthosilicate acid with various soluble organic and inorganic compounds [4]. It has been previously shown that the monomeric form of orthosilicate acid improves the coagulation efficiency of aluminum hydroxychlorides in the processes of water treatment of surface waters with high turbidity [5], due to the formation of a stable complex with an aluminum atom [6, 7]. Therefore, one of the important requirements for the selection of substances capable of stabilizing orthosilicic acid is environmental safety. Such substances include methane sulfonic acid, which corresponds to the concept of green chemistry [8].

In our previous experimental study [9], we demonstrated that different organic and inorganic acids stabilize orthosilicate acid solutions in different ways. In [10], it was theoretically shown that otosilicate acid can bind to a methanesulfonic acid molecule and form a cluster $H_4SiO_4 \cdot CH_3SO_3^-]$. In this work, it was of interest to find out the possibility of formation and structure of clusters with more methanesulfonic acid molecules per orthosilicate acid molecule. The aim of the work was to study the energy of intermolecular hydrogen bonds, geometric structure, and to compare the stability of orthosilicate acid clusters with different numbers of bound methanesulfonic acid anions.

I. Objects and methods of calculation

Quantum chemical modeling was performed using the software packages Gaussian 09 [11], AIM2000 [12], and AIMALL [13]. The clusters were optimized using the hybrid DFT functional B3LYP [14, 15]. Atoms were described using the basis set 6-311++G(d, p) [16], which

adequately describes cluster systems based on Silicon atoms [17, 18]. The influence of the aqueous environment was taken into account using the PCM polarization continuum model [19, 20]. From the beginning, modeling and optimization of clusters of the [$H_4SiO_4 \cdot nMS$] type were carried out, where MS is the methanesulfonate anion ($CH_3SO_3^-$), which forms hydrogen bonds with the molecule of orthosilicate acid (OSA), n is the number of MS molecules. To be able to compare the energies of the clusters, the same number of atoms was maintained in the system in the form of a cluster with the general composition [$H_4SiO_4 \cdot nMS$](MS)$_{(4-n)}$, where the conditional outer sphere is MS molecules that do not form any bonds with the OSA molecule , and the inner sphere is the opposite, respectively. For the optimized systems, the vibrational spectrum was calculated, based on the results of which the thermodynamic energy parameters were determined, such as the sum of the total electronic energy of the system with the appropriate thermodynamic corrections: to zero oscillations (E_{ZPE}); to Gibbs free energy (E_G); and enthalpy of the system (E_H). The total electronic energy of the system with a correction to zero oscillations (E_{ZPE}) was used to calculate the energy effects of cluster formation (ΔE_{ZPE}). For the optimized systems, the calculation of the effective charge of silicon atoms was also carried out according to the theory of natural orbitals (NBO) [21] and the calculation of frontier orbitals according to the same method as the optimization of the geometry of the systems, but using a different basis set – 6-311G(d, p) [22, 23]. Then the electron density distribution $\rho(r)$ was calculated using the QTAIM method [24]. The binding energy of hydrogen bonds was calculated using the Espinosa equation [25]: $E_b = 0.5 \cdot v(r) \cdot 2625.5$, where E_b is the binding energy, $v(r)$ is the potential energy density in the corresponding

critical point (3; –1), and 2625.5 is the conversion factor of the Hartree measurement unit in kJ/mol.

II. Results and discussion

In the process of modeling clusters of the type [$H_4SiO_4 \cdot nCH_3SO_3^-$], two conformations of OSA were considered. The first conformation (A) forms two hydrogen bonds between the hydrogen of the OH groups of the orthosilicate acid (OSA) and the oxygen atom with each MS molecule. For example, for [$H_4SiO_4 \cdot CH_3SO_3^-$] (A) (Fig. 1, a), hydrogen bonds with interatomic distances of 1.729 and 1.731 Å are formed with binding energies of –48.21 and –48.03 kJ/mol, respectively. And for [$H_4SiO_4 \cdot 2CH_3SO_3^-$] (A) (Fig. 1, b), two hydrogen bonds of 1.767 and 1.756 Å are formed with the first MS molecule, and 1.767 and 1.758 Å with the second. At the same time, the torsion angle of the H-O-O-H OSA for conformation (A) is small. For example, for [$H_4SiO_4 \cdot CH_3SO_3^-$] (A) (Fig. 1, a) it is 1.53°; for [$H_4SiO_4 \cdot nCH_3SO_3^-$] (A) (Fig. 1, b) it is 10.98 and 14.35°. For clusters of conformation (A), up to two methane sulfonate anions can be held in the inner sphere due to the limited number of OH groups of the CSA. Any attempts to attach a third or fourth MS molecule to the inner sphere resulted in the repulsion of MS to the outer sphere (Fig. 2).

The configuration (B) forms one hydrogen bond each with the OH group hydrogen and the methane sulfonate anion oxygen, and the second weaker hydrogen bond is formed between the OSA oxygen and the methyl group hydrogen of the methane sulfonate anion. For the cluster [$H_4SiO_4 \cdot CH_3SO_3^-$] (B), the value of the NO-OH torsion angle (at the site of the formation of the OC) is 131° (Fig. 3, a). When moving to the cluster
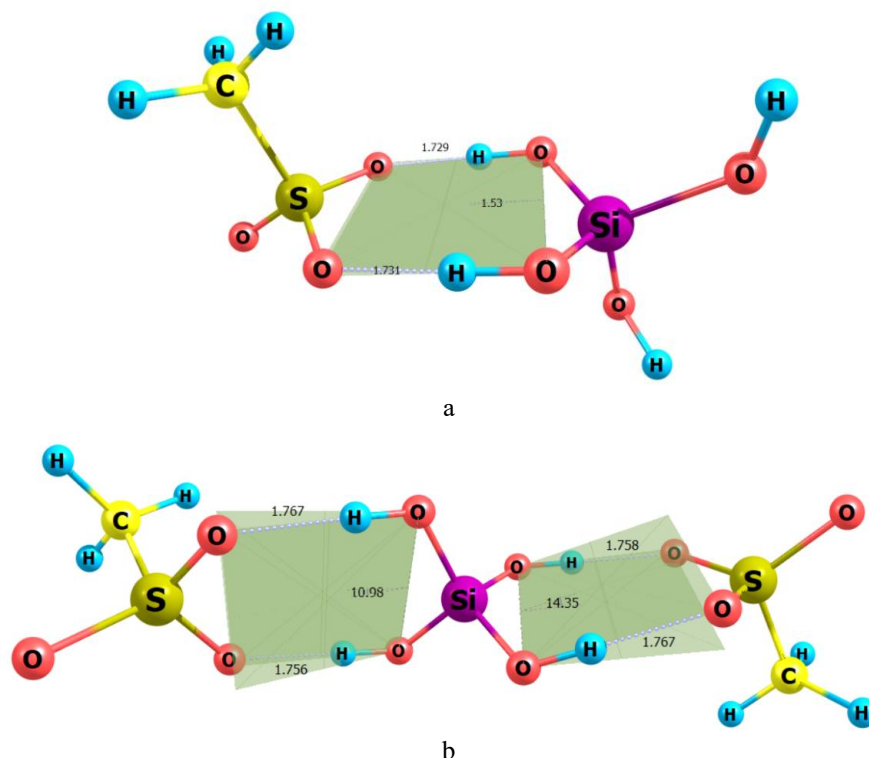

a

b

Fig. 1. Geometrical structure of clusters of conformation (A): a – [$H_4SiO_4 \cdot CH_3SO_3^-$]; b – [$H_4SiO_4 \cdot 2CH_3SO_3^-$].
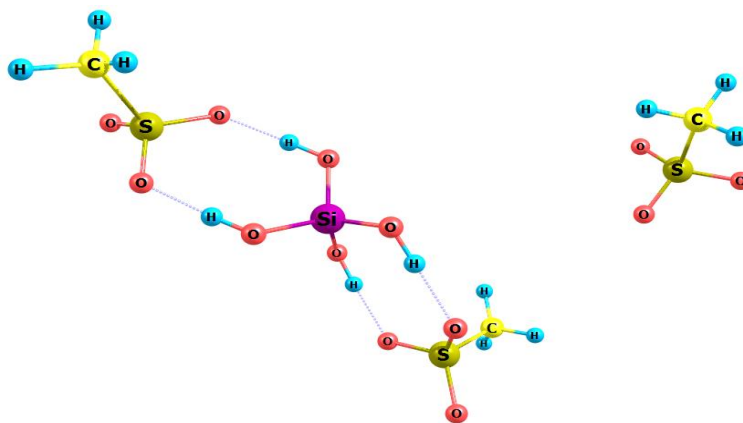
Fig. 2. Model of the cluster: $[H_4SiO_4 \cdot 2CH_3SO_3^-](CH_3SO_3^-)$ (A).

$[H_4SiO_4 \cdot 2CH_3SO_3^-]$ (B), the torsional angles of NO-OH range from 106° to 161°; for $[H_4SiO_4 \cdot 3CH_3SO_3^-]$ (B) from 110° to 151° (Fig.3,b); and for $[H_4SiO_4 \cdot 4CH_3SO_3^-]$ (B) from 105° to 150°, respectively.
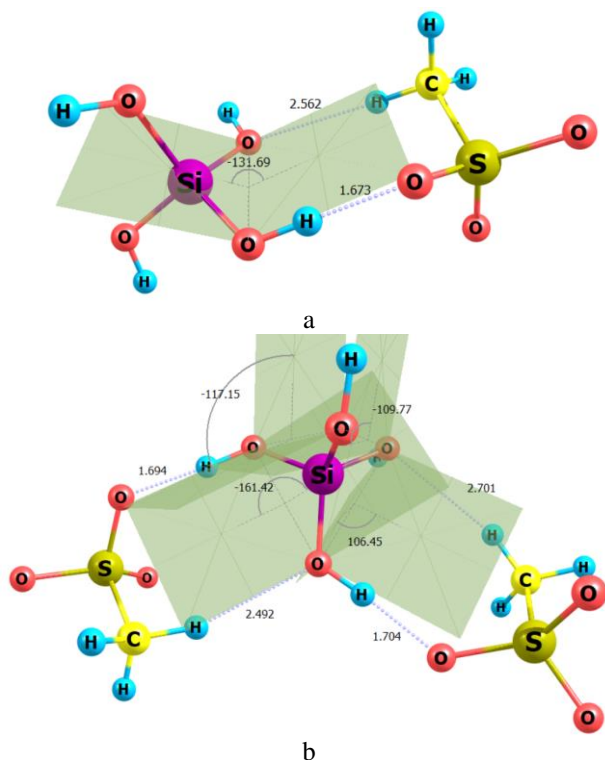

Fig. 3. Geometrical structure of clusters of conformation (B): a – $[H_4SiO_4 \cdot CH_3SO_3^-]$; b – $[H_4SiO_4 \cdot 2CH_3SO_3^-]$.

It can be seen that hydrogen bonds of different strengths are formed for configuration (B). For example, for $[H_4SiO_4 \cdot CH_3SO_3^-]$ (B) (Fig. 3, a), hydrogen bonds of 1.673 and 2.562 Å are formed with corresponding binding energies of –58.42 and –5.91 kJ/mol. In comparison with $[H_4SiO_4 \cdot CH_3SO_3^-]$ (B) in $[H_4SiO_4 \cdot 2CH_3SO_3^-]$ (B) (Fig. 3, b), the average value of the interatomic distances of the first and second hydrogen bonds increases, while the value of the binding energy of hydrogen bonds decreases accordingly: for E_b (SO⋯H) –54.37 and

–52.74 kJ/mol; for E_b (CH⋯OSi) –6.87 and –4.15 kJ/mol. And the same tendency of decreasing binding energy with increasing MS molecules is observed for all other clusters: for $[H_4SiO_4 \quad 3CH_3SO_3^-]$ (B) – $E_b^{average}$(SO⋯H) = –49.84 and $E_b^{average}$(CH⋯OSi) = –6.29 kJ/mol; for $[H_4SiO_4 \cdot 4CH_3SO_3^-]$ (B) – $E_b^{average}$(SO⋯H) = –46.40 and $E_b^{average}$(CH⋯OSi) = –6.42 kJ/mol.

It was found that a characteristic feature of all the studied clusters at the level of electron density distribution is the formation of an eight-membered cycle (S-O⋯H-O-Si-O-H⋯O) for all conformations (A) and a cycle (S-O⋯H-O-Si-O⋯H-C) for all conformations (B). This fact confirms the presence of a critical point (3; +1), which corresponds to the minimum electron density in the center of the cycle. Using the example of the cluster $[H_4SiO_4 \cdot CH_3SO_3^-]$ (B), it can be seen (Fig. 5) that a critical point (3; +1) is formed in the plane of the eight-membered cycle (depicted in red), and green dots correspond to saddle critical points (3;–1), and are the identifier of the chemical bond between atoms in the cluster.

The calculations of energy parameters for the clusters $[H_4SiO_4 \cdot nCH_3SO_3^-](CH_3SO_3^-)_{(4-n)}$ showed (Table 1) that the cluster $[H_4SiO_4 \cdot 4CH_3SO_3^-]$ has the lowest values of E_{ZPE}, E_G, E_H (highlighted in green), so it is the most stable system compared to other studied clusters

A linear dependence for all calculated energy parameters on the number of MS molecules is observed. The confidence coefficient for different energy parameters decreases in the series $E_{ZPE} \rightarrow E_G \rightarrow E_H$, and is 0.9956, 0.9662, 0.9469, respectively (Fig. 6). Therefore, further calculations of energy effects were analyzed using E_{ZPE} (Fig. 6. a).

The energy effect of sequential addition of MS molecules has a slight decrease. Thus, the addition of the first MS molecule to the OSA has the largest value of –27.48 kJ/mol (1), and the energy effect of the addition of the second, third, and fourth MS molecules has values of –23.28 and –19.85 and –17.28 kJ/mol, respectively. The total energy effect of the addition of all four MS molecules is –87.89 kJ/mol, which is only three times greater than the energy effect of the addition of one MS molecule.
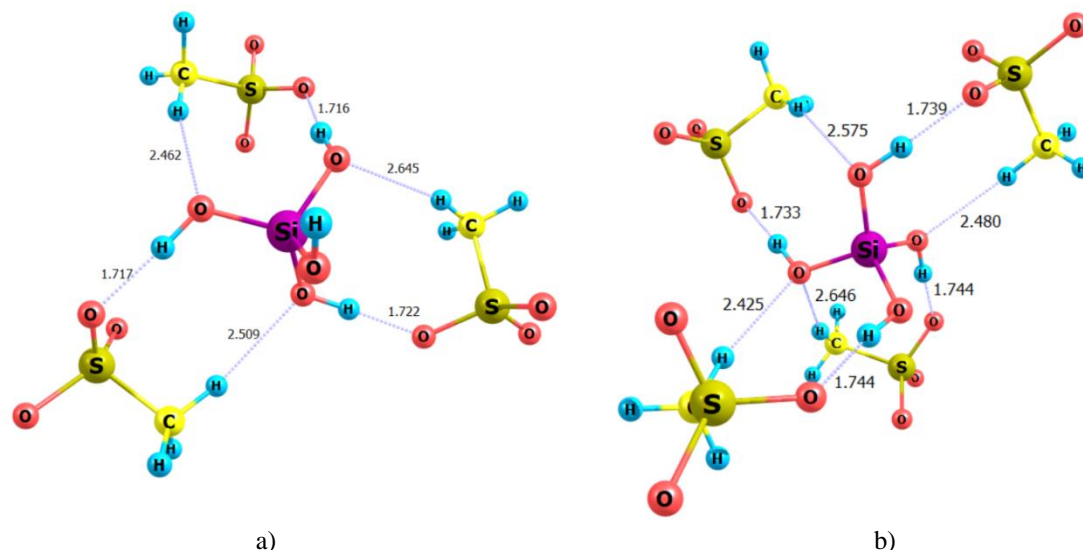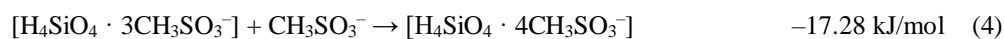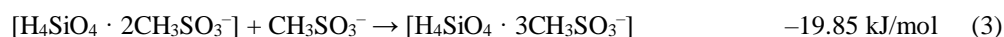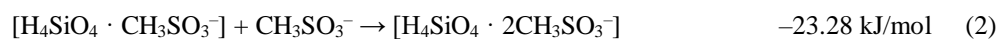
a)   b)

Fig. 4. Geometrical structure of clusters of conformation (B): a – [H$_4$SiO$_4$ · 4CH$_3$SO$_3^-$]; b – [H$_4$SiO$_4$ · 4CH$_3$SO$_3^-$].

$$H_4SiO_4 + CH_3SO_3^- \rightarrow [H_4SiO_4 \cdot CH_3SO_3^-] \qquad\qquad -27.48 \text{ kJ/mol} \quad (1)$$

$$[H_4SiO_4 \cdot CH_3SO_3^-] + CH_3SO_3^- \rightarrow [H_4SiO_4 \cdot 2CH_3SO_3^-] \qquad\qquad -23.28 \text{ kJ/mol} \quad (2)$$

$$[H_4SiO_4 \cdot 2CH_3SO_3^-] + CH_3SO_3^- \rightarrow [H_4SiO_4 \cdot 3CH_3SO_3^-] \qquad\qquad -19.85 \text{ kJ/mol} \quad (3)$$

$$[H_4SiO_4 \cdot 3CH_3SO_3^-] + CH_3SO_3^- \rightarrow [H_4SiO_4 \cdot 4CH_3SO_3^-] \qquad\qquad -17.28 \text{ kJ/mol} \quad (4)$$
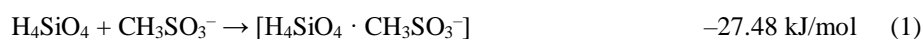
The calculated effective charges on the silicon atoms showed that the latter do not significantly change depending on the number of bound MS molecules and range from 2.318 to 2.320 Å. According to the calculations of the marginal molecular orbitals, it is clear that the highest occupied molecular orbital (HOMO) is concentrated on methanesulfonate anions, while the lowest unoccupied molecular orbital (LUMO) is concentrated in the center of the cluster where the OSA molecule is located (Fig. 5) Table 2 shows that the values of E_{gap} increase with the increase of bound MS molecules. Thus, the calculations of the maximum molecular orbitals
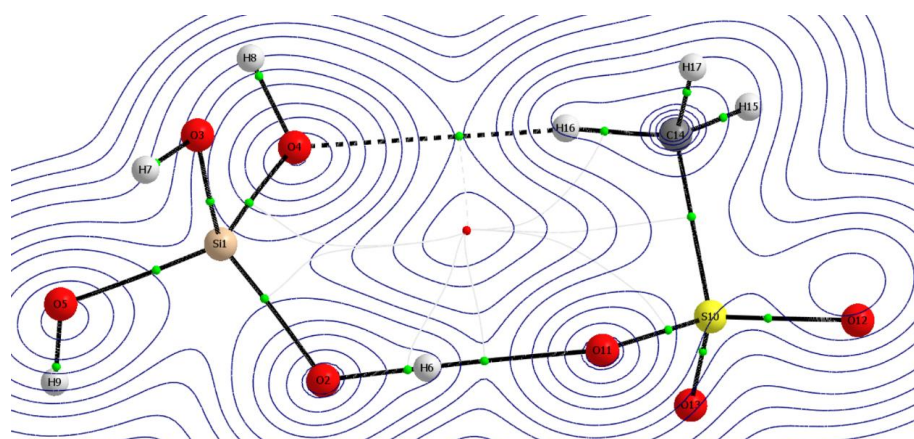

Fig. 5. Molecular graph of the cluster [H$_4$SiO$_4$ · CH$_3$SO$_3^-$] (B).

Table 1.

Energy parameters of the clusters [H$_4$SiO$_4$ · nCH$_3$SO$_3^-$](CH$_3$SO$_3^-$)$_{(4-n)}$ conformation (B)

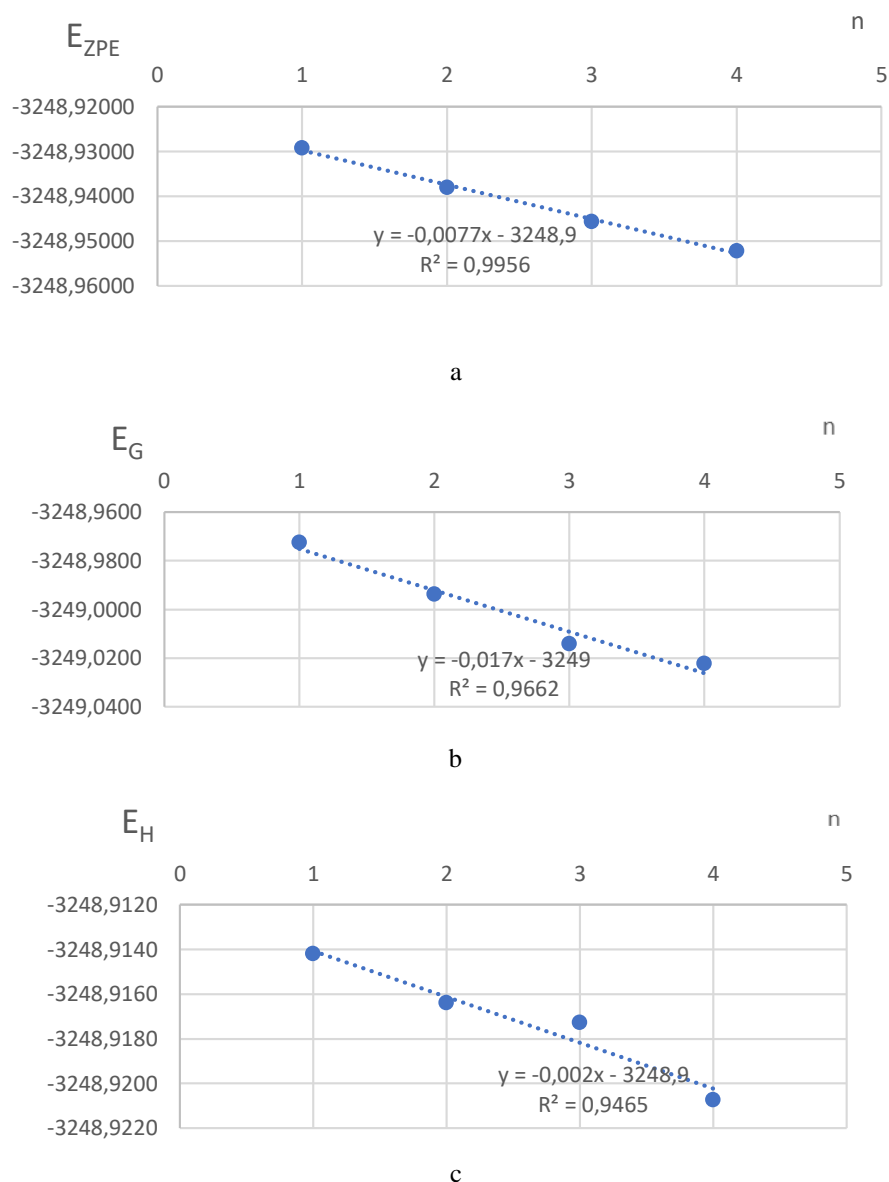| Clusters	$-E_{ZPE}$, kJ/mol	$-E_G$, kJ/mol	$-E_H$, kJ/mol
[H$_4$SiO$_4$ · CH$_3$SO$_3^-$](CH$_3$SO$_3^-$)$_3$	3248.92913	3248.97241	3248.91420
[H$_4$SiO$_4$ · 2CH$_3$SO$_3^-$](CH$_3$SO$_3^-$)$_2$	3248.93800	3248.99372	3248.91640
[H$_4$SiO$_4$ · 3CH$_3$SO$_3^-$](CH$_3$SO$_3^-$)	3248.94556	3249.01424	3248.91727
[H$_4$SiO$_4$ · 4CH$_3$SO$_3^-$]	3248.95214	3249.02230	3248.92074

a

b

c

Fig. 6. The dependencies of energy parameters on the number of MS molecules in the cluster $[H_4SiO_4 \cdot nCH_3SO_3^-](CH_3SO_3^-)_{(4-n)}$: $a - E_{ZPE}$, $b - E_G$, $c - E_H$.
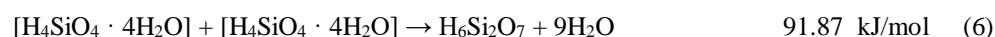
Table 2.

Calculations of frontier MOs for the clusters $[H_4SiO_4 \cdot nCH_3SO_3^-]$ of conformation (B)

Clusters	E_{HOMO}, eB	E_{LUMO}, eB	E_{GAP}, eB
$[H_4SiO_4 \cdot CH_3SO_3^-]$	–0.24929	0.01965	0.26894
$[H_4SiO_4 \cdot 2CH_3SO_3^-]$	–0.24728	0.02618	0.27346
$[H_4SiO_4 \cdot 3CH_3SO_3^-]$	–0.24507	0.03477	0.27984
$[H_4SiO_4 \cdot 4CH_3SO_3^-]$	–0.24296	0.03874	0.28170

show that the cluster $[H_4SiO_4 \cdot 4CH_3SO_3^-]$ is the most stable structure in aqueous solution among the studied clusters, which is consistent with the comparison data from the calculations of the energies of the systems.

The energy effects of the dimerization of the OSA and clusters based on it were calculated. It can be seen that according to reaction (7), the dimerization of CNTs in the composition of the cluster $[H_4SiO_4 \cdot 4CH_3SO_3^-]$ is quite energetically complicated in comparison with the dimerization (6) of the cluster $[H_4SiO_4 \cdot 4H_2O]$ by 60 kJ/mol.

$$H_4SiO_4 + H_4SiO_4 \rightarrow H_6Si_2O_7 + H_2O \qquad\qquad -23.40 \ \text{kJ/mol} \quad (5)$$

$$[H_4SiO_4 \cdot 4H_2O] + [H_4SiO_4 \cdot 4H_2O] \rightarrow H_6Si_2O_7 + 9H_2O \qquad\qquad 91.87 \ \text{kJ/mol} \quad (6)$$

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$$[H_4SiO_4 \cdot 4CH_3SO_3^-] + [H_4SiO_4 \cdot 4CH_3SO_3^-] \rightarrow H_6Si_2O_7 + 8CH_3SO_3^- + H_2O \quad 152.38 \text{ kJ/mol} \quad (7)$$

Conclusions.

The possibility of binding orthosilicate acid to different amounts of methanesulfonic acid anions was considered using quantum chemical modeling. It was demonstrated that methanesulfonic acid forms two hydrogen bonds with an orthosilicate acid molecule, regardless of the conformation of the cluster itself (two conformations with the symbols (A) and (B) were shown). Conformation (A) can bind up to two methanesulfonate anions at most, and conformation (B) – up to four. These conformations differed from each other by different values of the torsion angle (H-O-O-H) of the orthosilicate acid in the clusters. Based on the results of calculations of the energy parameters of the systems and the boundary molecular orbitals, it was found that the most stable cluster of orthosilicate acid with methanesulfonate anion is $[H_4SiO_4 \cdot 4CH_3SO_3^-]$. It was also found that a characteristic feature for all the studied clusters at the level of electron density distribution is the formation of an eight-membered cycle (S-O$\cdots$H-O-Si-O-H$\cdots$O) for all conformations (A) and a cycle (S-O$\cdots$H-O-Si-O$\cdots$H-C) for all conformations (B). The linear dependence of various energy parameters on the number of bound methanesulfonate anions is shown. The absence of a significant dependence of the effective charge from the silyl atom on the number of methanesulfonate anions in the inner sphere was also found. Thus, it has been theoretically demonstrated that methanesulfonate anion is able to stabilize orthosilicate acid and reduce the possibility of its dimerization.

Mandryka A.H. – PhD student at the Department of Inorganic Substances Technology and Ecology;
Pasenko O.O. – PhD in Engineering, Associate Professor of the Department of Inorganic Substances Technology and Ecology;
Vereshchak V.H. – Doctor of Technical Sciences, Professor of the Department of Inorganic Substances Technology and Ecology
Osokin Y.S. – PhD in Chemistry, Teacher chemistry and biology in Primus Inter Pares School.

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А.Г. Мандрика[1], О.О. Пасенко[1], В.Г. Верещак[1], Є.С. Осокін[2]

Моделювання кластерів ортосилікатної та метансульфонової кислоти у водному розчині

[1]*Український державний хіміко-технологічний університет, Дніпро, Україна,*
[2]*Primus Inter Pares School, Дніпро, Україна, osokin@cf.dnu.dp.ua*

В роботі з використанням квантово-хімічного методу моделювання була розглянута можливість зв'язування ортосилікатної кислоти з різною кількістю метансульфонат-аніонів. Було продемонстровано, що метансульфонова кислота утворює по два водневі зв'язки з молекулою ортосилікатної кислоти, в незалежності від конформації самого кластеру. За результатами розрахунків енергетичних параметрів систем та граничних молекулярних орбіталей, було встановлено, що найстабільнішим кластером ортосилікатної кислоти з метансульфонат-аніоном є [$H_4SiO_4 \cdot 4CH_3SO_3^-$]. Також було встановлено, що характерною особливістю для всіх досліджуваних кластерів на рівні розподілу електронної густини є утворення восьмичленного циклу (S–O···H–O–Si–O–H···O) та (S–O···H–O–Si–O···H–C). Також встановлено відсутність суттєвої залежності ефективного заряду від атома Силіцію від кількості аніонів метансульфонату у внутрішній сфері. Таким чином, теоретично продемонстровано, що метансульфонат-аніон здатний стабілізовувати ортосилікатну кислоту та зменшувати можливість її димеризації.

Ключові слова: ортосилікатна кислота; метансульфонова кислота; кластери; водний розчин; квантово-хімічне моделювання; енергія зв'язування; водневий зв'язок.