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ANALYSIS OF THE INTERACTION BETWEEN N-ACETYLNEURAMINIC ACID AND DISACCHARIDES ON SILICA SURFACE

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Nanocomposites based on biomolecules and highly dispersed silica are quite promising for use in many fields of biotechnology. There are many methods of obtaining such materials, in particular, adsorption from liquid or gas phases. Saccharides and their derivatives are present in the human body, they are involved in metabolic process, thus it is reasonable to use them while working with biomolecules. The work considers such disaccharides as sucrose, lactose and N-acetylneuraminic acid (NANA). Being a part of glycoproteins and glycolipids, NANA is also considered to be a carbohydrate. The main objective of the study was to study the ways of interaction of NANA on the disaccharide-modified silica surface. The methods of quantum chemistry have been used to find the probable structures of three-component adsorbtion complexes at molecular level and to clarify the mutual influence of these compounds in adsorbtion process. An analysis of the results of quantum chemical calculations shows that the adsorption of an anion of N-acetylneuraminic acid on silica surface is less likely than in its molecular form. Molecules of N-acetylneuraminic acid, disaccharides and silica form intermolecular complexes due to intermolecular hydrogen bonds between polar functional (mainly –OH) groups of the analytes. The sucrose dimer is 85.4 kJ/mol stronger than the lactose one. The sucrose molecule also forms a 38.1 kJ/mol stronger intermolecular complex with the N-acetylneuraminic acid molecule compared to a similar complex where lactose is used as a disaccharide. The highest energy (245.2 kJ/mol) is released when a silica cluster interacts with the intermolecular complex of N-acetylneuraminic acid and sucrose provided silica and the sucrose molecule are in a direct contact with each other. Therefore, as studies have shown, the adsorption of N-acetylneuraminic acid is possible if silica surface is pre-modified with disaccharides. The results of quantum chemical modeling confirm the obtained experimental data.

Keywords*: N-acetylneuraminic acid, silica surface, sucrose, lactose, adsorption, cluster approach, density functional theory method*

INTRODUCTION

Biodesign at the molecular level is a promising area of modern chemistry, including obtaining and elucidating the properties of nanomaterials based on silica and biomolecules. Such composites are used in cryopreservation of reproductive cells in veterinary medicine, and complexes with N-acetylneuraminic acid (NANA) are widely used in medicine as those that supply infected cells with drugs and as tumor markers [1–3].

The main objectives of this research were to study the ways of interaction of NANA with disaccharide-modified silica surface by experimental and quantum chemical methods, to find probable structures of three-component adsorption complexes at the molecular level and to elucidate the interaction of these compounds during adsorption.

Calculations show that the adsorption of monosaccharide molecules on silica surface is possible and give their location and the sequence of adsorption in a three-component system [4].

OBJECTS AND METHODS OF RESEARCH

The research materials are:

– highly dispersed silica (HDS) with a specific surface area of 300 m^2/g (Kalush Research and Experimental Plant of the Institute of Surface Chemistry of the National Academy of Sciences of Ukraine);

– sucrose (Reakhim, Kyiv), a non-reducing carbohydrate that contains residues of two monodisaccharides: *α-D*-glucose and *β-D*-fructose.

– lactose (Sigma, USA), a disaccharide that contains residues of two carbohydrates: glucose and galactose.

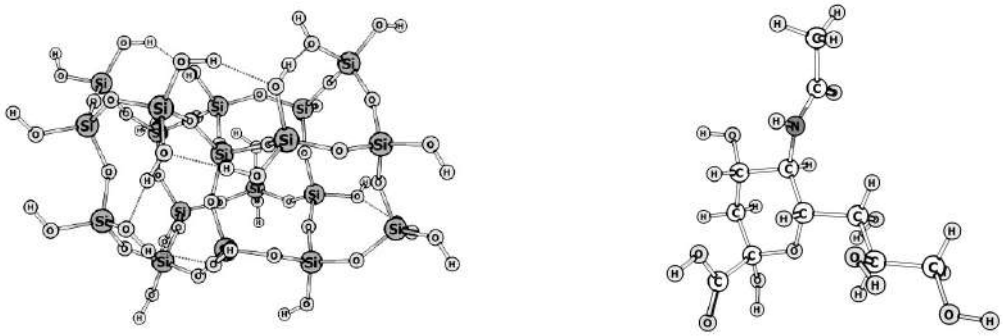
– N-acetylneuraminic acid (Sigma, USA) - sialic acid, which is a part of glycoproteins and glycolipids. It is located at the ends of their molecules and plays an important role in recognizing the components of the membrane cell environment.

The sucrose model shown in Fig. 1 *a* [7] was taken for the quantum chemical calculations. This model consists of residues of *D*-glucopyranose and *D*-fructofuranose interconnected by an oxygen bridge, and the lactose model is a disaccharide formed from residues of *D*-galacto-pyranose and *D*-glucopyranose (Fig. 1 *b*) [8].

A cluster consisting of 18 silicon-oxygen tetrahedra (Fig. 2 *a*) was used as a model of silica surface. This model was used in our previous work [4] where the interaction of silica with monosaccharides and N-acetylneuraminic acid was researched. It allowed us to compare energy characteristics calculation results of compounds in the present research with similar values calculated in the previous one [4]. The model of the molecular form of N-acetyl-neuraminic acid is presented in Fig. 2 *b*.

a *b*

Fig. 1. Equilibrium spatial structure of disaccharide molecules: *a* – sucrose, *b* – lactose



a *b*

Fig. 2. Models: *a* – silica cluster, *b* – molecular form of N-acetylneuraminic acid

Quantum chemical calculations were performed with GAMESS (US) program [9] by density functional theory (DFT) method with functional B3LYP [10, 11] and basis set 6-31G (d, p). Grimm variance correction D3 was adjusted [12, 13] within the polarization continuum model (PCM) [14, 15].

The value of the energy effect of proton transfer from the molecule of N-acetyl-neuraminic acid to the water molecule, i.e. the energy effect of electrolytic dissociation (ΔE_{dis}) of this acid in aqueous solution and on silica surface was calculated by the formula:

$$\Delta E_{dis} = E_{(ion.\ compl.)} - E_{(mol.\ compl.)}, \quad (1)$$

where $E_{(ion.\ compl.)}$ – is the total energy of an intermolecular complex consisting of an undissociated acid molecule and water molecules, $E_{(mol.\ compl.)}$ – is the total energy of an intermolecular complex consisting of a NANA anion, a hydroxonium cation, and water molecules.

Calculations of the adsorption energy (ΔE_{ads}) of one molecule of disaccharide on silica surface were performed according to formula (2):

$$\Delta E_{ads.} = E(_{ads.\ compl}) - ((E_{(surf)} + E_{(mol)}), \quad (2)$$

where $E_{(ads.\ compl)}$ is the total energy of the intermolecular complex, $E_{(surf)}$ and $E_{(mol)}$ are the

total energies of the silica cluster and the studied molecule, respectively.

The energy of intermolecular interaction between two identical molecules (sucrose and lactose) due to formation of dimers was calculated by formula (3):

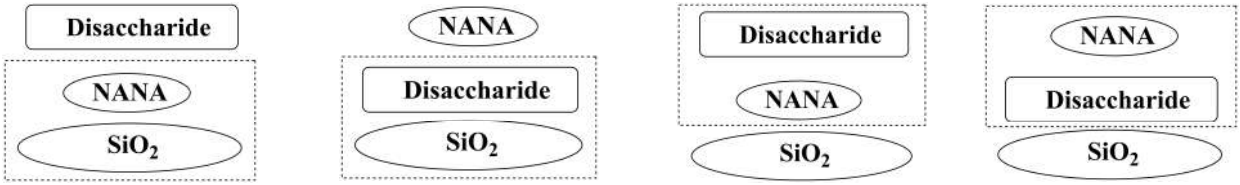
$$\Delta E_{dim.} = E_{(compl)} - 2E_{(mol)}, \quad (3)$$

where $E_{(compl)}$ is the total energy of the intermolecular complex of two identical molecules (dimer), $E_{(mol)}$ is the total energy of the molecule of the test compound.

The energy of formation of intermolecular complexes of NANA with disaccharides was calculated by formula (3), similar to the above described:

$$\Delta E_{int.\ react} = E_{(intermolec.\ compl)} - (E_{(NANA)} + E_{(disacch)}), \quad (4)$$

where $E_{(intermolec.\ compl.)}$ is the total energy of the intermolecular complex, $E_{(NANA)}$ and $E_{(disacch)}$ are the total energies of the NANA molecules and the test disaccharide, respectively.



Scheme 1 Scheme 2 Scheme 3 Scheme 4

Fig. 3. Possible types of interaction in a three-component system consisting of silica, NANA and disaccharides

To clarify the mutual influence on the adsorption of disaccharides and N-acetyl-neuraminic acid on silica surface, it is necessary to consider several variants of interactions in the three-component system (Fig. 3): silica - NANA - disaccharide; silica - NANA - disaccharide, according to similar schemes given in our previous research [4]. The Schemes 1 and 2 depicted above describe the interaction of a single molecule with the adsorbed complex. Namely, the Scheme 1 involves the interaction of a disaccharide molecule with a molecule of NANA, previously adsorbed on silica surface. The Scheme 2 shows the kinds of the NANA molecule interaction with the intermolecular disaccharide-silica complex.

The Schemes 3 and 4 schemes describe the interaction of the intermolecular disaccharide-NANA complex with a silica cluster. According to the Scheme 3, the intermolecular complex directly interacts with silica from the NANA side. In the Scheme 4, the interaction of the complex with silica occurs from the disaccharide, respectively.

RESULTS AND DISCUSSIONS

The results of experimental studies. The experiment [16] proves that unlike disaccharides (sucrose, lactose), monosaccharides (glucose, fructose) and N-acetylneuraminic acid (NANA) are not capable to be adsorbed on the hydroxylated surface of silica from the aqueous phase. This is due to the fact that silica surface in the studied pH range has a negative charge and NANA is an anion and at the used pH value (5.0) is also negatively charged. Therefore, a lactose molecule was used to separate a like-charged HDS surface from the anion NANA in space to reduce their electrostatic repulsion and to create a three-component system with silica, lactose and NANA. Quantum chemical calculations made it possible to predict the structures of complexes during the adsorption of these compounds on silica surface [17].

Nanocomposites are obtained in various ways, namely by adsorption from the liquid [5] and gas [6] phases. Nanocomposites were created on the basis of silica and disaccharides using adsorption at 20–23 °C. Adsorption time: 2 h with constant stirring, the ratio of solution: sorbent is 1:10. Centrifugation at 4000 rpm was used to separate the solid phase, and the amount of non-adsorbed sugar in the supernatant was determined using molybdate-sulfur solution [19].

It has been found that sucrose from the aqueous phase is capable to be adsorbed on silica surface. Working concentration of aqueous solutions of sucrose is 10^{-2}–10^{-3} mol/l. The adsorption isotherm has an S-shape (Fig. 4). It proves that the adsorbate molecules on the

surface of the carrier can be located in a chain (according to Parfit and Rochester) [20]. Therefore, it is assumed that silica surface contributes to the chain arrangement of sucrose molecules.

In Fig. 4. we can see that monomolecular adsorption with a saturation concentration of 12×10^3 mg/g follows at the initial stage of adsorption (in the range of concentrations 0–0.8 mg/ml). It means that during adsorption the first layer on silica surface is filled and then polymolecular adsorption begins [21].

Adsorption of lactose on silica surface was also performed by pH=5 adsorption method (concentration range – 0.25–2.5 mmol/g) where silica surface has a negative charge.

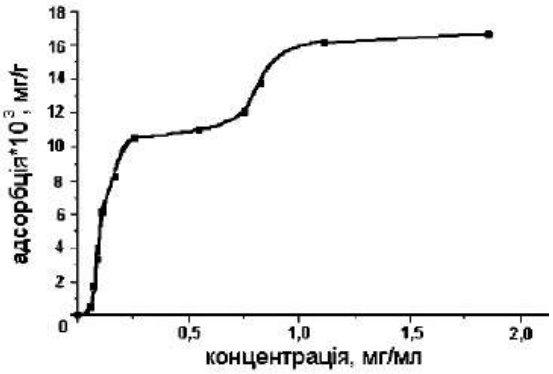
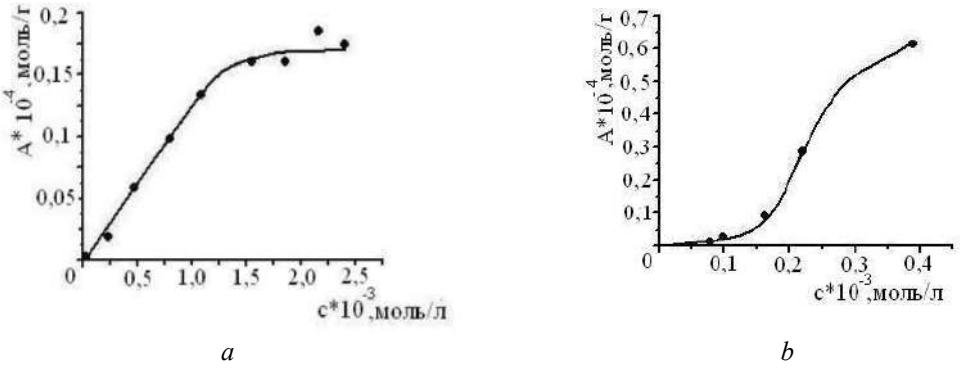


Fig. 4. Sucrose adsorption isotherm on silica surface



a *b*

Fig. 5. Isotherms of lactose adsorption on silica surface and adsorption of N-acetylneuraminic acid on the lactose-modified silica surface

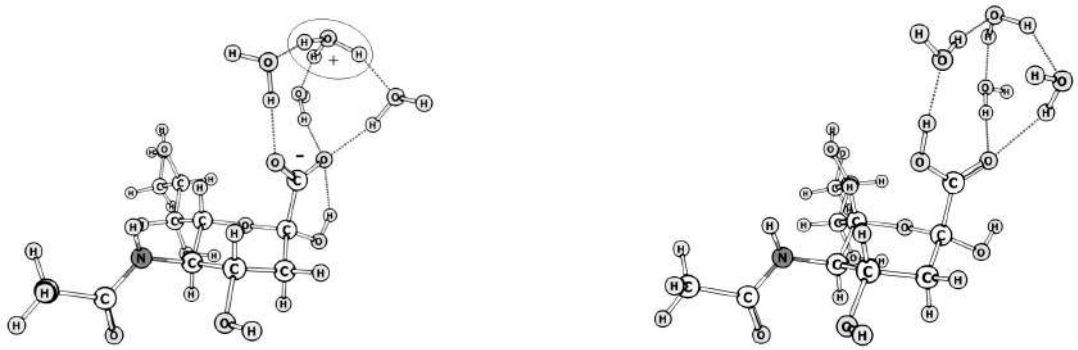
Fig. 5 *a* shows the isotherm of lactose adsorption on silica surface and Fig. 4 *b* shows the adsorption isotherm of NANA on the lactose-modified silica surface. According to Hills' classification, they correspond to L- and S-type, respectively, proved by literature data [22].

The results of quantum chemical calculations. Since N-acetylneuraminic acid is a rather strong acid with pK = 2.6 [23], in aqueous solution it can interact with disaccharides and silica in both molecular and dissociated states. Thus, first of all it was necessary to investigate the interaction of silica with NANA in molecular and dissociated form, and to elucidate the effect of surface silica on the dissociation of this acid. For this purpose, two NANA states were considered: the ionized state is a complex with separated charges (Fig. 6 *a*), consisting of an organic anion and a hydroxonium cation, which are stabilized by three water molecules, and a similar gross molecular complex consisting of a neutral NANA molecule with four water molecules (Fig. 6 *b*).

The analysis the results of of calculations shows that the energy effect of proton transfer from the carboxyl group of the NANA molecule to the water molecule, calculated by formula (1), is positive and is characterized by a fairly small

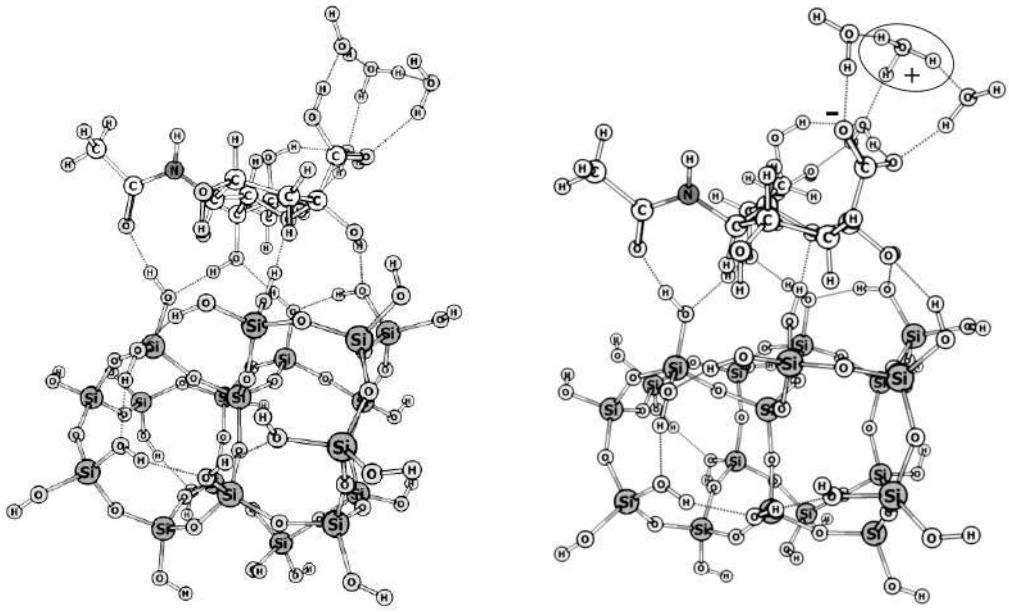
value (+0.32 kJ/mol). This indicates a fairly strong acidic property in comparison with silica [24], as well as with other organic acids like ascorbic acid [25].

To elucidate the effect of silica surface on the electrolytic dissociation of the NANA molecule, two complexes adsorbed on silica surface were designed similar to those discussed above. Fig. 7 shows that these two intermolecular complexes are bound to silica by six hydrogen bonds.



a *b*

Fig. 6. Equilibrium spatial structure of intermolecular complexes of a cluster of water molecules and N-acetylneuraminic acid in ionized (*a*) and molecular (*b*) forms



a *b*

Fig. 7. Equilibrium spatial structure of adsorption complexes of water molecules and N-acetylneuraminic acid in molecular (*a*) and ionized (*b*) forms on silica surface cluster

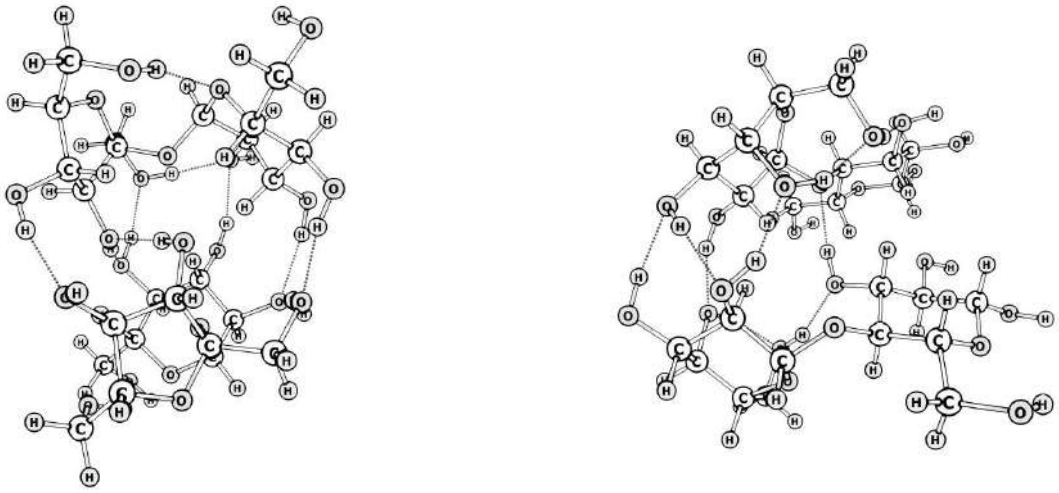
The calculations prove that the energy effect of proton transfer from the adsorbed NANA molecule to the water molecule is +11.4 kJ/mol, which is approximately 11 kJ/mol more than the same value of proton transfer without the presence of silica. Therefore, an analysis of the results of quantum chemical calculations has shown that the adsorption of NANA on silica surface reduces the capability to electrolytic dissociation of this molecule, and therefore suppresses its acidic properties.

The adsorption energy for the molecular complex (Fig. 7 *a*) on silica surface, calculated by formula (2), is -176.0 kJ/mol, and for a similar complex with separated charges, this value is -165.3 kJ/mol. Therefore, the NANA

anion on silica surface is adsorbed worse than the molecule. In this regard the adsorption complexes of the molecular form of NANA on silica surface and disaccharides will be considered further.

Then the energy of disaccharide dimer formation and their interaction with NANA on the silica surface was calculated.

Sucrose and lactose form dimers through hydrogen bonds between the hydroxyl groups of disaccharides (Fig. 8). In this case the results of the calculation by formula (3) prove that the energy effect of the formation of dimer (ΔE_{dim}) of sucrose is more than 85 kJ/mol greater in absolute value than the same value for lactose (Table 1) and is -255.6 kJ/mol compared to -170.2 kJ/mol for lactose.



a *b*

Fig. 8. Intermolecular complexes of disaccharides: *a* – sucrose dimer, *b* – lactose dimer

The values of dimer formation energy are much lower than previously obtained ones within the same method [4], similar values in the formation of monosaccharide dimers, for glucose they are -66.3 kJ/mol, and for fructose dimer -91.7 kJ/mol, respectively. But for the intermolecular complex of two molecules NANA ΔE_{dim} it is close to the same value for sucrose and lactose and is -188.2 kJ/mol [4].

This can be explained by the approximately identical size of the disaccharide molecules with NANA and the presence of more polar functional groups in their composition, which are capable to form hydrogen bonds, compared to monosaccharides.

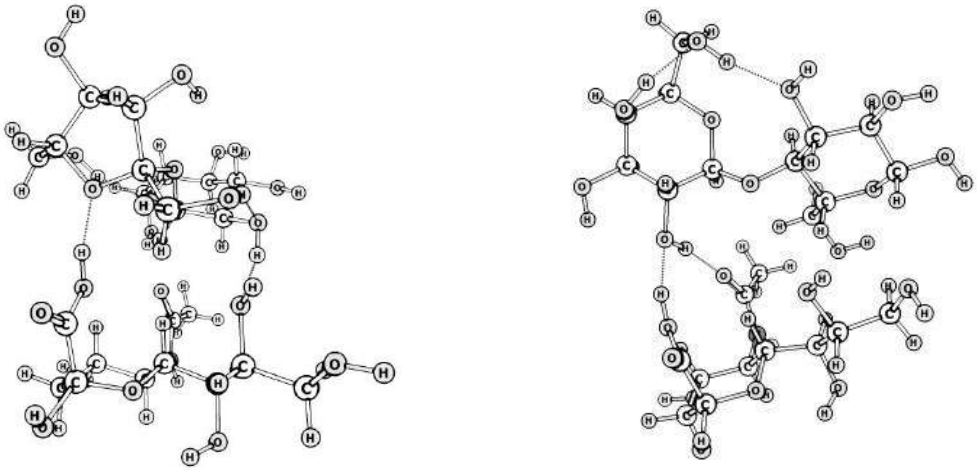
Next, it was necessary to study the energy and geometry parameters of the interaction of NANA with every single disaccharide. Fig. 9 presents intermolecular complexes that are formed when intermolecular hydrogen bonds take place. These bonds are formed due to carboxyl and hydroxyl groups of the NANA molecule and hydroxyl groups of disaccharides, as well as the glycosidic oxygen atom of the *D*-fructofuranose sucrose residue.

Analysis of the results of calculating the energy of intermolecular interaction of the NANA molecule with disaccharides according to formula (4) has shown (Table 1) that for the NANA-sucrose complex $\Delta E_{int.\ react}$ has a lower value (-178.8 kJ/mol), compared to a similar value for the NANA-lactose complex, which is -140.7 kJ/mol. This indicates that the sucrose molecule binds more strongly to the NANA molecule than lactose.

In modeling the interaction of disaccharides with silica surface the structures of intermolecular adsorption complexes of sucrose and lactose with a silica cluster were set. Fig. 10 shows that they are formed, like those discussed above, by the emergence of hydrogen bonds between the polar functional groups of disaccharides and a silica cluster.

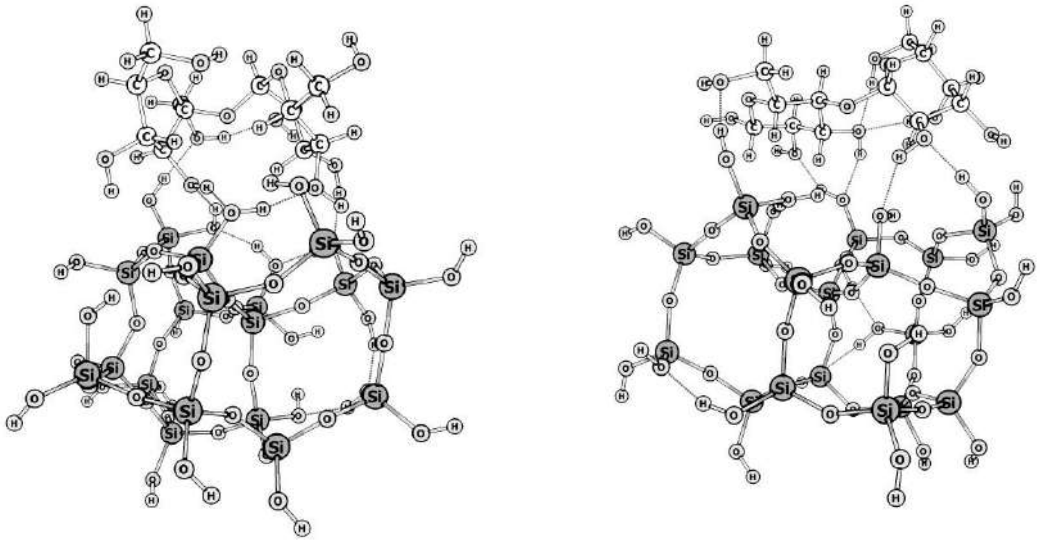
The calculations of the adsorption energy (ΔE_{ads}) made by formula 2 are presented in Table 1. It shows that the adsorption energy for the sucrose-silica complex has a lower value

(211.7 kJ/mol) compared to the similar value for the lactose-silica complex, where adsorption energy is 154.9 kJ/mol. Comparison of these values with the literary data for the adsorption of glucose (-161.0 kJ/mol), fructose (-174.8 kJ/mol), as well as for NANA (-163.2 kJ/mol) on silica surface [4], prove that among all four considered carbohydrates, sucrose is the best adsorbed on silica surface, and the value of NANA adsorption is slightly higher (8.3 kJ/mol) in absolute value in comparison with the similar value for lactose.



a *b*

Fig. 9. Intermolecular complexes of N-acetylneuraminic acid and disaccharides: *a* – sucrose, *b* – lactose



a *b*

Fig. 10. Adsorption complexes of silica with disaccharides: *a* – sucrose, *b* – lactose

Table 1. Energy of intermolecular interaction of disaccharides (kJ/mol)

Types of intermolecular complexes	Sucrose	Lactose
Dimers	-255.6	-170.2
Intermolecular complexes with NANA	-178.8	-140.7
Adsorption complexes with SiO_2	-211.7	-154.9

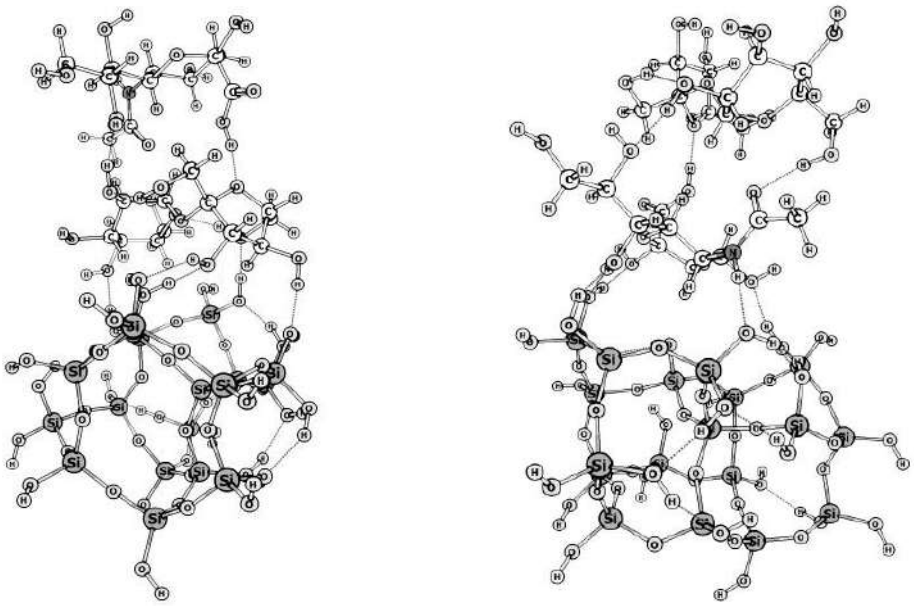
After considering the interaction of every single disaccharide molecule with NANA molecule, and the interaction of each studied compound with silica surface, it's time to consider the three-component systems (silica-disaccharide-NANA and silica-NANA-disaccharide).

Like in our previous research [4], four schemes of intermolecular interaction are considered here for these two three-component systems.

The sucrose was used to set the structures of two of these three-component systems shown in Fig. 10. In the first system, the sucrose molecule is directly bound by hydrogen bonds to the silica cluster, and the NANA molecule has no such bond with silica (Fig. 11 *a*). In the second system, the sucrose molecule has no hydrogen bond with silica, but is bound to the NANA molecule, which in its turn forms hydrogen bonds with silica surface (Fig. 11 *b*).

The calculation results are presented in Table 2. It shows that the smallest interaction in the case of sucrose is characteristic of scheme three (-194.4 kJ/mol), and the largest is found for scheme 4, the value of the interaction energy for which is -245.2 kJ/mol. For interaction schemes 1 and 2, this value is a middle ones they are -210.0 for scheme 1 and -212.2 kJ/mol for scheme 2, respectively. This means that from the point of view of thermodynamics interaction of sucrose with NANA in aqueous solution is more likely, and then the intermolecular complex on the side of sucrose interacts with silica.

Similar to the above three-component systems with sucrose, the structures with lactose are shown in Fig. 12. In this case, this figure shows that the number of hydrogen bonds between silica and intermolecular complexes is less than that for similar complexes in the case of sucrose.

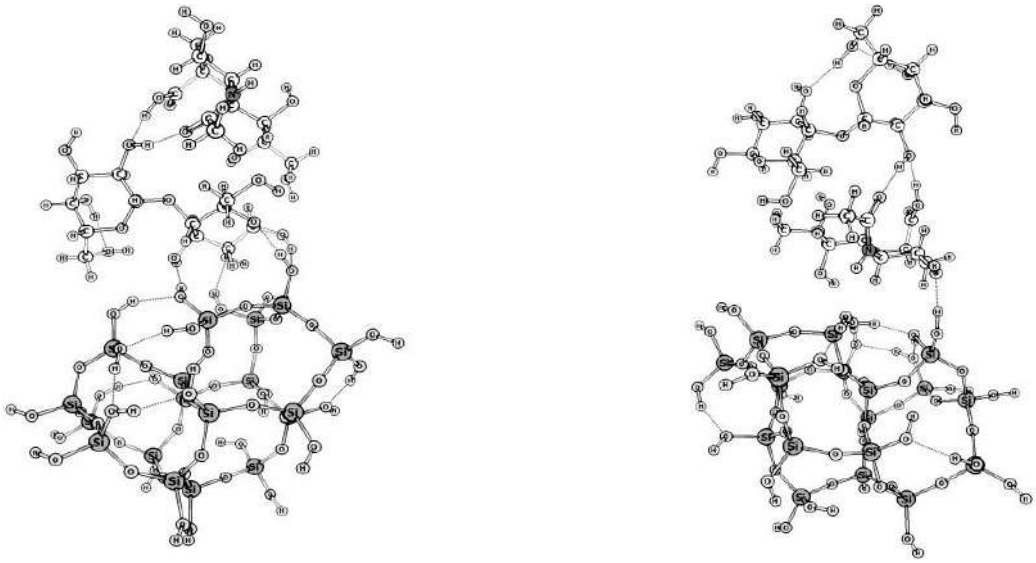


a *b*

Fig. 11. Three-component adsorption complexes: *a*–silica cluster, sucrose, N-acetylneuraminic acid; *b*–cluster of silica, N-acetylneuraminic acid, sucrose

Table 2. Energy of intermolecular interaction of disaccharides of NANA and silica (in kJ/mol) according to schemes 1–4

	Schemes			
	1	**2**	**3**	**4**
Sucrose	-210.0	-212.2	-194.4	-245.2
Lactose	-74.5	-113.9	-96.9	-128.1
Glucose [4]	-196.0	-160.9	-226.3	-188.9
Fructose [4]	-179.5	-104.0	-197.7	-133.9



a *b*

Fig. 12. Three-component adsorption complexes: *a* –silica cluster, lactose, N-acetylneuraminic acid; *b* – silica cluster, N-acetylneuraminic acid, lactose

The calculation results of the interaction energy according to the four schemes for complexes with lactose are also presented in Table 2. It shows that for all four schemes, the use of lactose leads to lower absolute values for the interaction energy compared to similar values for sucrose. In particular, according to Scheme 1, the interaction energy is the lowest of all the cases considered earlier and is -74.5 kJ/mol. And the highest energy (-128.1 kJ/mol) is released during the interaction of the NANA-lactose complex with the silica cluster from the lactose side.

In addition, comparing these values with similar literature data [4], it turns out that when using monosaccharides glucose and fructose in three-component systems, the interaction energies are higher in absolute values compared to the presence of lactose in similar complexes.

Analyzing the data in Tables 1 and 2, and comparing them with the literature data of adsorption of glucose on silica surface (-161.0 kJ/mol), fructose (-174.8 kJ/mol) and NANA (-163.2 kJ/mol) [4] we can see that not all carbohydrates contribute to the adsorption of NANA on silica, in particular it refers to fructose, and the carbohydrate that best promotes the adsorption of NANA from those considered is sucrose.

CONCLUSIONS

A analysis the results of quantum chemical calculations shows that the adsorption of anion of N-acetylneuraminic acid on silica surface is less likely than in its molecular form. Molecules of disaccharides, N-acetylneuraminic acid and silica cluster form triple complexes due to intermolecular hydrogen bonds between polar functional (mainly –OH groups) of the substances that are the subjects of the research. Sucrose is better adsorbed on silica surface (ΔE_{ads} = -211.7 kJ/mol) compared to the adsorption of lactose (-154.9 kJ/mol). The sucrose dimer is 85.4 kJ/mol stronger than the lactose dimer. Also, the sucrose molecule forms an intermolecular complex with the N-acetylneuraminic acid molecule wich is 38.1 kJ/mol stronger compared to a similar complex where lactose is used as a disaccharide. The highest energy of 245.2 kJ/mol is released when interacting of the intermolecular complex of N-acetylneuraminic acid and sucrose with a silica cluster, while silica and the sucrose molecule are in a direct contact with each other.

Thus research shows that the adsorption of N-acetylneuraminic acid is possible if silica surface is pre-modified with disaccharides. The results of quantum chemical calculations confirm the obtained experimental data.

Аналіз взаємодії N-ацетилнейрамінової кислоти із дисахаридами на поверхні кремнезему

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Нанокомпозити на основі біомолекул та високодисперсного кремнезему досить перспективні для використання в багатьох галузях біотехнології. Методів одержання таких матеріалів є немало, зокрема, це адсорбція із рідкої або із газової фаз. Сахариди і їхні похідні присутні в людському організму, вони беруть участь у метаболізмі, тому для роботи з біомолекулами доречно використовувати саме такі речовини. У роботі розглянуті дисахариди – сахароза, лактоза та N-ацетилнейрамінова кислота (NANA), яка є частиною глікопротеїнів та гліколіпідів, також є вуглеводом. Основною задачею дослідження було вивчення шляхів взаємодії NANA на модифіковану дисахаридами поверхню кремнезему. За допомогою методів квантової хімії встановлені ймовірні структури трикомпонентних адсорбційних комплексів на молекулярному рівні і з'ясовано взаємний вплив цих сполук при адсорбції. Результати аналізу квантовохімічних розрахунків свідчать, що адсорбція на поверхні кремнезему аніона N-ацетилнейрамінової кислоти менш ймовірна, в порівнянні з її молекулярною формою. Молекули дисахаридів N-ацетилнейрамінової кислоти та кремнезему утворюють міжмолекулярні комплекси за рахунок міжмолекулярних водневих зв'язків між полярними функціональними (в основному –ОН) групами досліджуваних речовин. Димер сахарози на 85.4 кДж/моль міцніший за димер лактози. Також молекула сахарози утворює на 38.1 кДж/моль міцніший міжмолекулярний комплекс з молекулою N-ацетил-нейрамінової кислоти в порівнянні із аналогічним комплексом, в якому як дисахарид використано лактозу. Найбільша енергія виділяється (245.2 кДж/моль) при взаємодії з кластером кремнезему міжмолекулярного комплекса N-ацетилнейрамінової кислоти і сахарози, при цьому безпосередньо контактують кремнезем і молекула сахарози. Отже, як показали дослідження, адсорбція N-ацетилнейрамінової кислоти можлива, якщо поверхню кремнезему попередньо модифікувати дисахаридами. Результати квантовохімічного моделювання підтверджують одержані експериментальні дані.

Keywords: *N-ацетилнейрамінова кислота, поверхня кремнезему, сахароза, лактоза, адсорбція, кластерне наближення, метод теорії функціоналу густини*

Анализ взаимодействия N-ацетилнейраминовой кислоты с дисахаридами на поверхности кремнезема

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Нанокомпозиты на основе биомолекул и кремнезема – это очень перспективное направление во многих отраслях биотехнологий. Методов получения таких материалов немало, в частности адсорбция из жидкой и газообразной фаз. Сахариды и их производные присутствуют в человеческом организме, они принимают участие в работе метаболизма, именно этим объясняется их использование для работы с биомолекулами. В работе рассматривается дисахариды – сахароза и лактоза, а также N-ацетилнейраминовая кислота (NANA), которая является частью гликолипидов и гликопротеинов и тоже углевод.

Основной задачей исследования было изучение взаимодействия NANA с модифицированной дисахаридами поверхностью кремнензема. С помощью методов квантовой химии установлены вероятные структуры трехкомпонентных адсорбционных комплексов на молекулярном уровне и изучено влияние этих соединений при адсорбции. Анализ результатов квантовохимических расчетов говорят о том, что адсорбция на поверхности кремнезема аниона N-ацетилнейраминовой кислоты менее вероятна в сравнении с ее молекулярной формой. Молекулы дисахаридов, N-ацетилнейраминовой кислоты и кремнезема образуют межмолекулярные комплексы за счет межмолекулярных связей между полярными функциональными (в основном –ОН) группами исследуемых веществ. Димер сахарозы на 85.4 кДж/моль более прочный, чем димер

лактозы. Также молекула образует на 38.1 кДж/моль более прочный межмолекулярный комплекс с молекулой N-ацетилнейраминовой кислоты по сравнению с аналогичным комплексом, в котором использована лактоза как дисахарид. Наибольшая энергия (245.2 кДж/моль) выделяется при взаимодействии с кластером кремнезема межмолекулярного комплекса N-ацетилнейраминовой кислоты и сахарозы, при этом непосредственно контактируют кремнезем и молекула сахарозы.

Следовательно, как показали исследования, адсорбция N-ацетилнейраминовой кислоты возможна, если поверхность кремнезема предварительно модифицировать дисахаридами. Результаты квантовохимического моделирования подтверждают полученные экспериментальные данные.

***Ключевые слова**: N-ацетилнейраминовая кислота, поверхность кремнезема, сахароза, лактоза, адсорбция, кластерное приближение, метод теории функционала плотности*

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