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QUANTUM-CHEMICAL MODELING OF MOLECULAR COMPLEXES STRUCTURE IN "URONATIC POLYESACHARIDES – Ca^{2+}" SYSTEM

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ABSTRACT *Quantum-chemical modeling of the process of ionotropic gelling in systems of uronate polysaccharides (high-guluronate sodium alginate and low-esterified pectin) with calcium is carried out. Calculation the interaction of active functional groups of uronate polysaccharides with calcium ion shows the possibility of this process passage with the formation of calcium-guluronate ($CaGul_4$), calcium-galacturonate ($CaGal_4$) and calcium-guluronate-galacturonate ($CaGal_2Gul_2$) chelate complexes.*
The process of interaction occurs when the carboxyl and hydroxyl groups of the uronate polysaccharides are chemically bound to the calcium ion. It was established that calcium-guluronate complex has an eight binding centres with calcium whereas calcium-galacturonate and calcium-guluronate-galacturonate complexes have four binding centres.
This article describes the binding centres in systems that are considered by ionotropic gel formation. This clearly illustrated the spatial atoms arrangement in the systems of individual polysaccharides and their combination; location and value of bond lengths, values of torsion and valence angles. Presented quantum-chemical models are allowed to estimate chemical activity of fragments macromolecular structures during ionotropic gelation. This makes it possible to predict the amount of external bound water, calculate the optimum proportions of substances for the formulation of rational food recipes.
The fact of the ionotropic gelation in the combined system "alginate-pectin-Ca" was installed on the basis of the obtained models and their geometric characteristics. In this case the chelate complexes $CaGul_2Gal_2$ was formed. It is stable during storage, more plastic and soft in contrast to $CaGul_4$ and stronger than $CaGal_4$.
Keywords*: alginate; pectin; complex formation; quantum-chemical modeling.*

КВАНТОВО-ХИМИЧЕСКОЕ МОДЕЛИРОВАНИЕ СТРУКТУР МОЛЕКУЛЯРНЫХ КОМПЛЕКСОВ В СИСТЕМЕ «УРОНАТНЫЕ ПОЛИСАХАРИДЫ – Ca^{2+}»

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АННОТАЦИЯ *Проведено квантово-химическое моделирование процесса ионотропного гелеобразования в системах уронатных полисахаридов (альгината натрия высокогулуронатного и пектина низкоэтерефицированного) с кальцием. Расчет взаимодействия активных функциональных групп уронатных полисахаридов с ионом кальция показывает возможность прохождения данного процесса с образованием хелатных комплексов кальций-гулуронатного, кальций-галактуронатного и кальций-гулуронат-галактуронатного.*
Процесс взаимодействия осуществляется за счет химического связывания карбоксильных и гидроксильных групп уронатных полисахаридов с ионом кальция. Установлено, что кальций-гулуронатный комплекс имеет восемь центров связывания с кальцием, а комплексы кальций-галактуронатный и кальций-гулуронат-галактуронатный имеют по четыре центра связывания.
В статье приводится описание центров химического связывания в рассматриваемых системах при реализаии принципа ионотропного гелеобразования. Наглядно представлено пространственное расположение множества атомов в системах отдельных полисахаридов и их комбинации; расположение и величины длин связей, значения торсионных и валентных углов. Представленные квантово-химические модели позволяют оценить химическую активность фрагментов структур макромолекул в случае протекания химических процессов ионотроплоного гелеобразования и дает возможность спрогнозировать количество внешнесвязанной воды, рассчитать оптимальные соотношения веществ для составления рациональных рецептур пищевых продуктов.
На основании полученных моделей и их геометрических характеристик был установлен факт протекания процесса ионотропного гелеобразования в комбинированной системе «альгинат-пектин-Са». В этом случае, образовался хелатный комплекс $CaGul_2Gal_2$, устойчивый в ходе хранения, более пластичный и мягкий в отличии от $CaGul_4$ и более прочный в отличии от $CaGal_4$..
Ключевые слова: *альгинат; пектин; комплексообразование; квантово-химическое моделирование.*

Introduction

Modern representation of food systems based on quantum-chemical modeling, allows obtaining the following results, important for the technological process organization:

1) derive an optimal ratio of the recipe components during the creating of food compositions;

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2) choose the most appropriate conditions for the chemical potential realization of the large macromolecules reactive sites, such as proteins and polysaccharides;

3) carry out diagnostics of different binding centers on the possibility of the chemical, van der waals interaction, hydration and mass transfer processes without costly investment into the experimental part;

4) obtain a general idea of the nutritional components and water role in the food compositions under consideration, for subsequent recommendations of chemical and physicochemical processes stabilization, associated with quality and safety indicators.

This article discusses systems based on sodium alginate (with an increased content of guluronate residues) and pectin (low esterified amidated) with realization of calcium ions chemical potential in various interaction with the remainders of uronic acids.

Calcium, as the most promising binding agent, and under consideration uronate polysaccharides, as widely used substances for obtaining gel-like systems with valuable food properties and technological characteristics, form firmly bound structures in food systems. These structures allow stabilizing the processes of moisture mass transfer and keep it to 30% when passing from the phase of the hydrogel to the xerogel [1].

Nowadays significant relevance is the study of polysaccharide compositions based on sodium alginate and pectin with other polysaccharides. For example, the authors [2] monitored the adsorption properties of the sodium alginate matrix with the participation of guar gum. The article [3] describes the molecular mechanism of lysozyme adsorption to a chemically modified alginate-guar matrix. New biodegradable and antibacterial edible films based on alginate hydrochloride and biguanidine chitosan are described in the article [4]. In the materials of the scientific publication [5] describe microgel of silylated (hydroxypropyl) methyl cellulose, which is considered as a multimodal system for the joint encapsulation of drugs. A group of scientists received alginate fibers coated with chitosan and described their antibacterial effect. [6].

The most obvious advantages are mixed pectin-alginate gels, structured by calcium ions [7, 8].

However, it should be noted, that systems based on this composition remain poorly research, although they have a significant economic effect when used in various technologies [9-12].

Objects

The purpose of this work is the detailed elaboration of theoretical study the features of molecular complexes equilibrium structures, which are implemented in the system «uronate polysaccharides – Ca^{2+}» by means of *ab initio* quantum chemistry methods.

Statement of the main material

Quantum chemical modeling is the method of obtaining the molecule electron energy and its wave function, which does not depend on the size and structure of the macromolecule.

It must be borne in mind three determining factors before the construction of a quantum chemical model. Namely, to select the components of the mathematical model, carry out a decision procedure and choose an atomic basis. Thus, to determine the method of obtaining the electron energy and the wave function [13].

The wave function is meant density matrix in density functional theory. It should be noted that this method does not describe any particular chemical system and can be applied to a molecule of any size and to any molecular structure and to any type of chemical binding. [14, 15].

Quantum-chemical models $CaGal_4$, $CaGul_4$, $CaGul_2Gal_2$, presented on the Figure 1 a-c were obtained on the basis of this.

Named images confirm the uniqueness of the Schrödinger equation solution for a given nuclei configuration, electron and spin states of the molecule. This solution is as close as possible to the objects under study, in particular, alginate-pectin-calcium complexes. Beside this, the presented models are applicable to a larger system, taking into account random molecular structures also.

The presented models require elaboration. Semi-empirical calculation methods were used for this. It is most expedient to continue calculations by the method M062x. It is necessary that several additional principles are fulfilled:

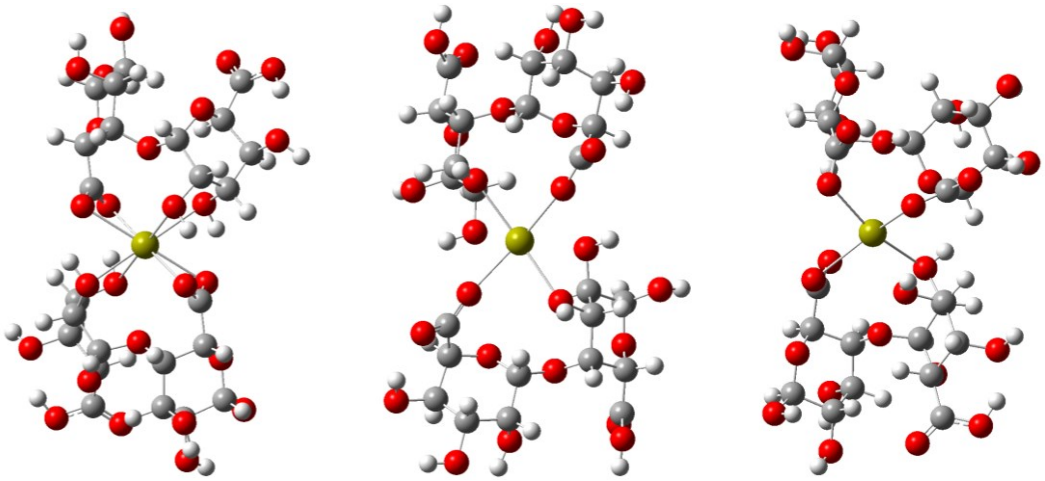
1. The results obtained for a system consisting of a minimum molecules set at an infinite distance from each other must correspond to the sum of the results obtained for isolated molecules of this system.

2. Energy, determined by this method, is the upper limit of the electron equation exact solution. The refinements, which were carried out by semi-empirical methods, made it possible to obtain smaller values of the energy than the obtained by molecular mechanic methods models.

Geometric parameters of chelate complexes “uronate polysaccharides – Ca^{2+}” that isolated from Z-matrices for optimized molecules of $CaGal_4$, $CaGul_4$, $CaGul_2Gal_2$ given in Table 1. Subsequently, using the theory of the density functional in the approximation B3LYP with the following modifications: M06, M062X, peculiarities the conformational transformations of uronate polysaccharides complexes with calcium were studied.

The lengths of bonds, torsion angles and valence angles were considered as geometric parameters.

Concerning the construction of macromolecular structures, in particular uronate polysaccharides, it is fair to say, that in Table 1 the characteristics of the complexes are visually represented: the lengths of the calcium ion with polysaccharides coordination bonds, torsion and valence angles.



a ***b*** ***c***

Fig. 1 – Models of stable calcium-uronate systems: ***a*** *– tetrahuluronate calcium ($CaGul_4$);* ***b*** *– tetragalacturonate calcium ($CaGal_4$);* ***c*** *– diguluronotadigalacturonate calcium ($CaGul_2Gal_2$)*

Table 1 – Geometric parameters of the system «uronate polysaccharides – Ca^{2+} chelate complexes»

		Complex							
		$CaGul_4$				$CaGal_4$		$CaGul_2Gal_2$	
		n	d	n	d	n	d	n	d
Length of bond Ca-O_n, Å		12	2.54038	53	2.54156	30	2.46918	38	2.53946
		78	2.52733	37	2.52801	12	2.42611	8	2.49132
		79	2.49019	38	2.49077	72	2.46897	55	2.48009
		49	2.48383	8	2.48322	54	2.42532	75	2.43800
		w-x-y-z				w-x-y-z		w-x-y-z	
Torsion angles $H_w – C_x – O_y – C_z$, ^{0}	φ	76-65-50-43		-61.15840		36-26-13-2	46.61303	79-69-56-45	-101.31086
		35-24-9-2		-61.15783		78-68-55-44	46.63952	35-24-9-2	-52.91515
	ψ	52-43-50-65		22.59891		1-2-13-26	20.04796	44-45-56-69	-6.15302
		11-2-9-24		22.59878		43-44-55-68	19.94151	11-2-9-24	15.11548
Valence angles $O_n – Ca – O_m$, ^{0}		n-m				n-m		n-m	
		12-37		114.60009		12-30	76.79737	75-55	76.07383
		8-38		115.46188		72-54	76.77659	38-8	106.73409
		78-53		114.58527		-	-	-	-
		79-49		115.44966		-	-	-	-
		49-38		94.79095		72-12	99.95322	75-38	85.60411
		54-37		92.60015		54-30	99.70507	55-8	99.93691
		78-12		92.63874		-	-	-	-
		79-8		94.79806		-	-	-	-

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Results and discussion

In the model of the complex $CaGul_4$ all links are equal with a small deviation within the permissible error 2,54038 ± 0.05716 Å.

Considering the model of the system $CaGal_4$, the values of the calcium bonds lengths with the oxygen atoms of the nearby carboxyl and hydroxyl groups have found a similar tendency. An average value of the bond length is 2,51283 Å with permissible deviations within ± 0.04386 Å. Comparing these indicators during the examination of the complex $CaGul_2Gal_2$, the average value of the bond length is somewhat smaller. This may indicate greater homogeneity and lower voltage of the binding atoms and more stable position. Thus, the average value of the bond length within the permissible error is 2,43800 ± 0.04386 Å.

Estimating the value of the bond length between the residues of uronic acids of polysaccharides with calcium in the complex $CaGul_2Gal_2$, it can be noticed, that these values for alginate and pectin have shifted towards the averaging. This is absolutely correct and natural as a result of the binding energies distribution in the system.

Torsion angles of the glycosidic bond were taken (as example of the system $CaGul_2Gal_2$) angle φ for atoms H_{76}-C_{65}-O_{50}-C_{43} and angle ψ for atoms H_{52}-C_{43}-O_{50}-C_{65} with quantitative characteristics - 101.31086 and - 6.15302 Å respectively (Fig. 2). It is worth noting, that torsion angles for chains of different polysaccharides are very different from each other and the difference is 48.39571 and 21.2685 Å.

At the same time in the systems $CaGal_4$ and $CaGul_4$, torsion angles φ and ψ have very similar meanings: 46.62623±0,0132 Å and -61.158115±0,00028 Å respectively.

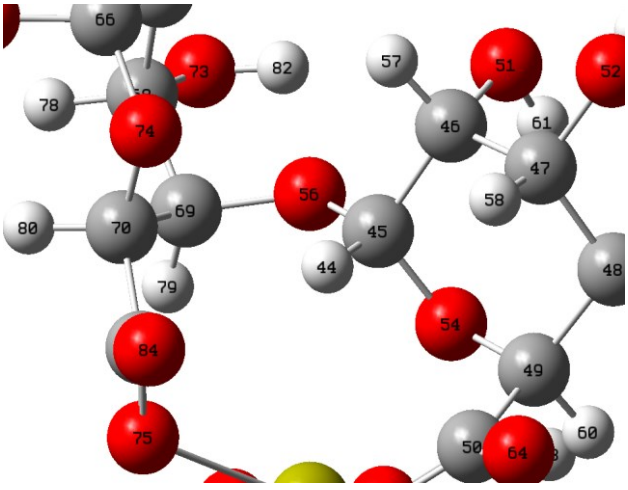

Fig. 2 – Fragment of the model $CaGul_2Gal_2$ with the notation of torsion angles φ and ψ ($H_w - C_x - O_y - C_z$)

Significant differences in torsion and valence angles in the system model $CaGul_2Gal_2$ connected with the geometry of uronate polysaccharides dimers. Guluronate remains have a more spatial structure, but galacturonate are more linear. In both structures ionotropic gel formation with the calcium ions participation proceeds successfully, as in the case of homogeneous uronate systems (alginate or pectinic).

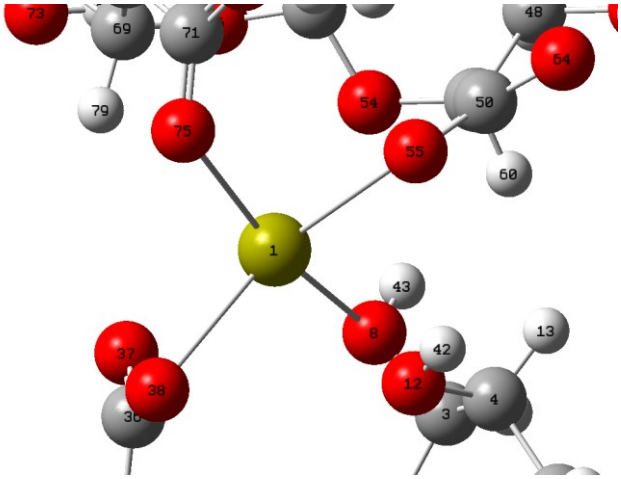

Fig. 3 – Fragment of the model $CaGul_2Gal_2$ with the notation of valence angles O_n-Ca-O_m

The valence angle with Ca, formed in the field of one ugonate polysaccharide and various, given on Fig. 3 (as example of the angle O_{79}-Ca-O_{49} and angle O_{79}-Ca-O_{12}).

Conclusions

It is of fundamental importance for understanding the chemistry of the ionotropic gel formation in systems of such polysaccharides, as low esterified amidated pectin and high-guluronate sodium alginate and their compositions, are the spatial arrangement of the set of atoms in these systems; the magnitude and location of bond lengths; values of torsion and valence angles. All of this in a case allows estimating the chemical activity of fragments macromolecules structures in the case of the ionotropic gel formation. This makes it possible to predict the amount of out-bound water, to calculate the optimum proportions of substances for the rational food recipes.

The fact of the ionotropic gel formation in a combined system “alginate-pectin-Ca” was established based on the obtained models and their geometric characteristics.

Chelate complex $CaGul_2Gal_2$, which formed, stable during storage, more plastic, softer as opposed to $CaGul_4$ and stronger than $CaGal_4$.

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АНОТАЦІЯ *Проведено квантово-хімічне моделювання процесу іонотропного гелеутворення в системах уронатних полісахаридів (альгіната натрія високогулуронатного і пектина низькоетерифікованого амідованого) з кальцієм. Розрахунок взаємодії активних функціональных груп уронатних полісахаридів з іоном кальцію пояснює можливість протікання даного процеса з утворенням наступних хелатних комплексів: кальцій-гулуронатного ($CaGul_4$), кальцій-галактуронатного ($CaGal_4$) та кальцій-гулуронат-галактуронатного ($CaGal_2Gul_2$).*

У статті повідомляється про те, що процес взаємодії здійснюється за рахунок хімічного зв'язування карбоксильних та гідроксильних груп уронатних полісахаридів з іоном металу. Встановлено, що кальцій-гулуронатний комплекс має вісім точок зв'язування з іоном кальцію, а комплекси кальцій-галактуронатний та кальцій-гулуронат-галактуронатний – по чотири. Описані довжини зв'язків, величини торсійних кутів та кутів O_n-Ca-O_m в одержаних хелатних комплексах.

Ключові слова: *альгінат; пектин; комплексоутворення; квантово-хімічне моделювання.*

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