

Guidelines for Authors

The Journal 'Herald of Technological University' publishes original theoretical, experimental and computational research papers from leading experts working in various fields currently being developed in Kazan National Research Technological University, scientific and educational institutions, industrial enterprises of the Republic of Tatarstan, the Russian Federation and abroad, as well as scientific reviews, the subject matter of which falls under the sections of the Journal:

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The file is named by the first author's last name and numbered.

3. Supporting documents shall include:

1) the text of the article signed by all co-authors, who by their signatures agree with the order of authorship in the title and confirm their contribution to the results presented in the article;

2) drawings, including photos, graphics, quality not less than 300 dpi, each as a separate jpeg or png file;

3) expert opinion on the possibility of publication in the open press, approved by the head of the relevant organization;

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4. The text of the article should be printed in the editor "Word", page parameters: upper margin 2 cm, lower margin - 1.5 cm, left margin - 1.75, right margin - 2 cm each, header - 1.0 cm, footer - 1.5 cm; font of the text of the article - Times New Roman Cyr 10 pt at one interval.

The font of keywords, abstract, references and information about authors - 9 pt; subscripts and superscripts - 10 pt Arial font. The paragraph indent is 0.5 cm. Key phrases of the text can be

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Review articles are sent to the Editorial Board of the Journal, as a rule, upon prior agreement with the Editor-in-Chief of the Journal and/or his/her deputies. When preparing review articles, the authors should take into account the following:

a) at least one of the authors of the review article must have his/her own publications on the subject of this article in reputable scientific journals indexed either in the List of VAK RF, or in Web of Science, or in Scopus; **at least 2 such publications** must be presented in the list of references for this review article;

b) the content of the review article should, among other things, also cover the achievements of recent years in this field of science, published both in Russian and foreign scientific literature (mainly in journals indexed in Web of Science and/or Scopus); at that, the total number of works cited in such an article (and, accordingly, references in the list of references to the article) should be at least 40. References to abstracts of local conferences and mass citations to conference proceedings are highly undesirable;

c) the so-called author's reviews, which systematize, analyze and summarize the works published mainly by the authors of the review article, may also be submitted for publication in the Journal; in this case, however, the authors must convincingly justify (in the cover letter to the Journal editorial board or in the introductory part of the article) that they develop a unique scientific direction in the relevant branch of science and hold leading positions in this direction.

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6. The text of the article should contain initial (including literature) data and the purpose of the work, for works of experimental nature - the experimental part (reagents, equipment, basic techniques), results and their discussion, list of references. Units of measurement and terminology recommended by IUPAC should be followed. All used symbols and abbreviations should be deciphered at the first mention of them in this article. Fractional parts of numbers are separated from whole numbers by a dot.

Duplication of data in the text, tables, figures, and their use in tables not discussed in the text of the literature data is not allowed.

7. The use of figures should be dictated by the need for a clearer understanding of the material presented and should not be an end in itself. One article should contain **no more than 5 (five) figures** (with obligatory reference to each of them in the text of the article). Figure with division into (a) and (b) parts is considered as Fig.1 and Fig.2. Each figure should have a format not more than 5x8 cm and in a form suitable for direct reproduction in printing. Figures may include brief numeric or alphabetic notations (numbered from left to right or clockwise) in a font appropriate to the rest of the text; the size of any notations in the figures should be chosen within 12-14 pt. The format of the figure should be chosen with respect to the image presented to avoid significant free margins. Figures should be included in the file, preferably immediately after the first mention of them in the text of the article. Captions to figures should contain the word "Fig." (space), figure number in Arabic numerals, dash, space, title with a capital letter (without a dot at the end of the sentence).

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The numbering and inclusion in the list of all literary sources mentioned in the article is mandatory. References to articles in print are not allowed. An article that does not contain references to literary sources will not be accepted for further consideration.

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Д. П. Романова, К. А. Романова, Ю. Г. Галяметдинов

QUANTUM-CHEMICAL MODELING OF STRUCTURE AND PHYSICO-CHEMICAL PROPERTIES OF MODIFIED PECTIN

Keywords: quantum-chemical modeling, modified pectin, density functional theory, IR spectroscopy.

Distinctive physicochemical and pharmacological properties of modified pectin, such as effective penetration into the bloodstream, powerful pro-inflammatory and profibrotic actions, determine its application in medicine for the treatment of cardiovascular and renal diseases, various inflammatory processes, to improve neurological health and prevent premature aging. Of particular note is its potent anti-cancer effect. It is also used as a flocculant in water purification; in mining and processing of minerals; in drilling to strengthen the walls of wells; as a superabsorbent; in agriculture. The physicochemical properties of pectin are directly related to its structure. In order to predict the structure and properties of compounds often resort to quantum-chemical modeling, which allows to study the physicochemical properties of a substance before its synthesis. However, there are limited works dealing with modeling the structure and properties of modified pectin. Therefore, in this work, an optimal approach to quantum chemical modeling of acrylamide-modified citrus pectin was searched for. The structure of the monomeric link of the polymer and its IR spectrum were calculated using several quantum chemical methods and basis sets. To evaluate the adequacy of the calculations, the calculated vibrational frequencies were compared with experimental data, which allowed us to establish the structure of the monomeric link and to find out that the modified pectin has a cyclic structure. As a result of comparing the calculated data with experimental data, the density functional theory method with PBE functional and 6-31G(d,p) basis set was proposed as the optimal quantum-chemical approach to modeling the structure and IR spectrum of modified pectin.

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КВАНТОВО-ХИМИЧЕСКОЕ МОДЕЛИРОВАНИЕ СТРОЕНИЯ И ФИЗИКО-ХИМИЧЕСКИХ СВОЙСТВ МОДИФИЦИРОВАННОГО ПЕКТИНА

Ключевые слова: квантово-химическое моделирование, модифицированный пектин, теория функционала плотности, ИК-спектроскопия.

Отличительные физико-химические и фармакологические свойства модифицированного пектина, такие как эффективное проникновение в кровоток, мощное противовоспалительное и профиброзное действия, определяют его применение в медицине для лечения сердечно-сосудистых и почечных заболеваний, различных воспалительных процессов, для улучшения неврологического здоровья и предотвращения преждевременного старения. Особого внимания заслуживает его мощное противораковое действие. Также он используется в качестве флокулянта при очистке воды; при добыче и переработке полезных ископаемых; при бурении для усиления стенок скважин; в роли суперабсорбента; в сельском хозяйстве. Физико-химические свойства пектина напрямую зависят от его строения. Для того, чтобы предсказать структуру и свойства соединений зачастую прибегают к квантово-химическому моделированию, позволяющему изучить физико-химические свойства вещества до проведения его синтеза. Однако существует ограниченное число работ, посвященных моделированию строения и свойств модифицированного пектина. Поэтому в данной работе был произведен поиск оптимального подхода к квантово-химическому моделированию модифицированного с помощью акриламида цитрусового пектина. Произведен расчет строения мономерного звена полимера и его ИК-спектра с использованием нескольких квантово-химических методов и базисных наборов. Для оценки адекватности проведенных расчетов вычисленные колебательные частоты сравнивались с экспериментальными данными, что позволило установить строение мономерного звена и выяснить, что модифицированный пектин имеет циклическое строение. В результате сравнения расчетных данных с экспериментальными в качестве оптимального квантово-химического подхода к моделированию строения и ИК-спектра модифицированного пектина был предложен метод теории функционала плотности с функционалом PBE и базисным набором 6-31G(d,p).

Introduction

In this age of polymers, there is no limit to the diversity of these compounds. Organic polymers and oligomers form an important class of modern materials that exhibit many attractive properties such as high elasticity, etc.,,,,,,

Literature

1. K. A. Romanova, Y. G. Galyametdinov, *Herald of Technological University*, **23**, 9, 5-8 (2020).
- 2.
- 15.

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