

Guidelines for Authors

Bulletin of the Technological University publishes original articles with experimental, theoretical, and computational research in different fields currently being developed at the university, scientific and educational institutions, industrial enterprises of the Republic of Tatarstan, the Russian Federation and abroad by leading university experts.

The following Manuscript Submission Requirements Checklist is provided to assist authors in the initial submission of their manuscript to *Bulletin of the Technological University*:

1. Authors should deliver 1 hardcopy of the manuscript signed by all the authors and 1 electronic copy to the journal's Editorial Board (to Head of Editorial Board of the Bulletin of Technological University Raziya Gusmanovna Romanova; E-mail: romanova_rg@mail.ru; Visiting address: Karl Marx str., 68, Kazan, Building A of the Kazan National Research Technological University (KNRTU), Room 335; Postal address: KNRTU, Karl Marx str., 68, Kazan, 420015, Russia)

2. Accompanying documents should include (1 copy each):

- Expert Opinion on the possibility of publishing the article in the open press (for articles in the area of natural sciences)

- a Certificate of Verification of the article by the Antiplagiat Program (while the degree of originality of the work in the part where the results of the study are presented should be at least 75%)

3. The computer version of the article should be drawn up in the form of a single file (two-lane version), including the UDC index, the initials and surnames of the authors (including the English spelling), the title of the article (in Russian and English), annotations in Russian and English languages (at least 200 WORDS), keywords (in Russian and English); full text and formulas, a list of cited literature (**at least 15 sources**), tables and, if possible, figures, information about the authors in Russian and English. **The file is named by the last name of the first author.**

4. The text should be typed in the Microsoft Word with the following page layout parameters: top margin of 2 cm, bottom margin of 1.5 cm, left margin of 1.75 cm, right margin of 2 cm each, Top and bottom headers are located in a distance of 1.0 cm and 1.5 cm from the page's top and bottom, respectively; The Times New Roman Cyr font with a size of 10 points and a single interval between the lines are used for typing the article's main text; A font size of 9 points is used for typing the abstract, keywords, literature references, and authors' data. Superscripts and subscripts are typed using the 10-points Arial font. Every paragraph is indented by 0.5 cm. The key phrases in the text may be italicized. The use of bold fonts, underlining, line spacing that is different from single spacing, and also empty spaces for indenting the paragraph are not allowed. Page numbers appear in the center of a bottom header.

Regular Articles should not exceed a volume of 10 pages including figures and tables.

Review Articles are published by the preliminary agreement with the editorial board. Authors are encouraged to consider the following when writing review articles:

a) At least one of the authors of the review article must have his own publications on the topic of this article in authoritative scientific journals, indexed either in the List of the Higher Attestation Commission of the Russian Federation, or in the Web of Science, or in Scopus; at the same time, at least 3 such publications should be presented in the list of references to this article;

b) The content of the review article, among other things, should also cover the achievements of recent years in this field of science, published both in Russian and foreign scientific literature, while the total number of cited works (and, accordingly, references in the list of references to the article) should be at least 40. At the same time, references to abstracts of any conferences are highly undesirable;

c) The author's reviews, in which the systematization, analysis and generalization of works published mainly by the authors of the review article are carried out, can also be submitted for publication in the journal; in this case, their authors must convincingly justify (in a cover letter to the editorial office of the journal or in the introductory part of the article) that they are developing a unique scientific direction in the relevant field of science and occupy leading positions in it.

5. Mathematical and chemical symbols in the formulas and equations, and superscript and subscript indices in the article's main text and in the figures are typed with using the 10-point Arial font. *Since the journal's layout is two-column, formulas* presented in the article should be placed in one column, i.e. their size should not exceed 5 × 8 cm.

6. In the article, it is desirable to adhere to the following order of presentation of the material. At the beginning there are UDC indices, initials and surnames of authors, title in Russian in capital letters, keywords in Russian, annotation in Russian; initials and surnames of authors, title in English in capital letters, keywords in English and annotation in English. Annotations and keywords are in italics. The text of the article should contain the initial (including literature) data and the purpose of the work; for experimental work: the experimental part (reagents, equipment, basic techniques), results and their discussion, list of references. The units of measurement and terminology recommended by IUPAC should be adhered to. All used symbols and abbreviations should be decrypted. Fractional parts of numbers should be separated by a commas.

Data in the text, tables, and figures should not duplicate each other, as well as using the literature data, which are not discussed in the main text, in tables and figures are not allowed.

7. The use of figures should be dictated by the need for a clearer understanding of the presented material. The publication may include **no more than 5 figures** (references to each figure should be present in the main text of the article). The (a) and (b) parts of a figure are considered as two separate figures (Fig.1 and Fig.2). Each **figure should not exceed a size of 5 × 8 cm**, and its format should be suitable for direct reproduction. Figures may include non-highlighted short

digital or letter symbols (numbered from the left to the right or clockwise) typed using a font that corresponds to the main text; a size of any symbols in the figures are chosen within 12–14 points. The figures should be formatted in such a way that no significant free space remains in the margins. It is desirable to incorporate figures into the main file (preferably immediately after the specified referring). Figure captions are composed as follows: the word ‘Fig.’, blank space, a figure’s number in numerals, dash, blank space, and figure’s caption started by a capital letter (without a period in the end).

8. The publication may include **no more than 3 tables**. Tables are given in the following form: the word ‘Table’ in the top left corner without indentation, a blank space, table’s number in numerals (if there are more than one table), dash, blank space, table’s caption started by a capital letter. Cell contents should be centered. **The table width should not exceed 8 cm**. If the table occupies more than one page, a line with the table column numbers sequenced from the left to the right appears below the table column titles on the first page, the second and subsequent pages begin with the word ‘Table’, a blank space, table’s number, blank space, the word ‘continuation’, period, and then the table with the corresponding column numbers in the first line is continued. Tables with a size less than one page should not be broken up into parts. The cell sizes and the table as a whole should be minimized as much as possible.

Only necessary numerical data are included in the tables. The numerical data should be processed statistically and according to metrology (units of measurements, error, etc. should be specified). Referring to tables in the article’s main text is mandatory. It is desirable to incorporate tables also into the main file, preferably immediately after the specified referring.

9. In exceptional cases, if the fulfillment of the requirements for the formatting of formulas, tables and figures leads to a distortion of the information provided, it is possible to arrange them across the width of one page with the subsequent formatting of the text in accordance with the Guidelines.

10. The cited literature is numbered in the order of mentioning, the reference number in the text is placed in square brackets. The list of references is placed in the end of the article and typed without paragraph indentions in accordance with the **Instructions for Design of References** (as given below). **The number of links in the article should be at least 15**.

Numbering and inclusion of all literature references mentioned in the article are obligatory. References to the articles which are in press are not allowed. A manuscript that does not list of references will not be accepted for further consideration.

11. After the list of references on the last page of the article, it is required to give **personal data of the authors**, as follows: the first, middle, and last names, science degree, position, department (laboratory, division), the name of institution, e-mail (with full translation of this information into **English**).

12. Manuscripts that do not meet any requirement of the Guidelines for Authors are returned to the authors. Upon re-submission of such manuscript, the deadline for its submission is updated.

13. A period of no more than one week is given to authors for finalizing the article after the editorial revision. The editorial board reserves the right to select materials on the competitive basis at the stage of preparation of the journal’s next issue.

14. The authors bear responsibility for the correct presentation of materials and usage of special terminology. The article’s galley proofs are not given to the authors for reviewing.

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Manuscripts, as well as a scanned Expert Opinion on the possibility of publishing the article in the open press and data on the verification of the article by the Antiplagiat Program (must accompany every manuscript submission), must all be submitted in electronic form for initial consideration by the Head of the Editorial Board Raziya Gusmanovna Romanova (vestnik@corp.knrtu.ru), Ph.D. in Chemistry, Associate Professor of the Department of Analytical Chemistry, Certification and Quality Management, KNRTU.

An example of the layout for the first page of the article is presented below.

UDC 535.37:544.164

D. P. Romanova, K. A. Romanova, Yu. G. Galyametdinov

QUANTUM-CHEMICAL SIMULATION OF THE STRUCTURE AND IR-SPECTRUM 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 pro-fibrotic effects, determine its application in medicine for the treatment of cardiovascular and renal diseases, various inflammatory processes, to improve neurological health and prevent premature aging. Its powerful anti-cancer effect deserves special attention. It is also used as a flocculant in water purification; in the extraction and processing of minerals; while drilling to strengthen the walls of wells; in the role of superb sorbent; in agriculture. Physicochemical properties of pectin directly depend on its structure. In order to predict the structure and properties of compounds, one often uses quantum-chemical simulation, which makes it possible to study the physicochemical properties of a substance before its synthesis. However, there is a limited number of works devoted to simulation of the structure and properties of modified pectin. Therefore, in this work, a search was made for an optimal approach for quantum-chemical simulation of citrus pectin modified with acrylamide. The calculation of the structure of the monomer unit of the polymer and its IR-spectrum by several quantum-chemical methods and basic sets has been performed. To assess the adequacy of the calculations, the obtained vibrational frequencies were compared with experimental data, which made it possible to establish the structure of the monomer unit and find out that the modified pectin has a cyclic structure. As a result of comparing the calculated data with the experimental ones, the density functional theory method with the PBE functional and the 6-31G (d, p) basis set was proposed as an optimal quantum-chemical approach for simulation of the structure and IR-spectrum of modified pectin.

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

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 провоспалительное 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 выявить, 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

В наш век полимеров многообразие этих соединений нет предела. Органические полимеры и олигомеры образуют важный класс современных материалов, которые демонстрируют множество привлекательных свойств, таких как высокая эластичность,

References

1. К. А. Романова, Ю. Г. Галяметдинов, *Вестник технологического университета*, **23**, 9, 5-8 (2020).

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1. Starting from January, 2012, the bibliographic information for all the common literature sources, i.e. articles, books, inventions, dissertations, and meeting papers (conferences, symposia, etc.), references to which are present in the journal should be given in the following uniform order:

1.1. For articles:

In Journals and other **Periodicals** (1) Initials and Surnames of all the authors given in the order appeared in the article in its original language, (2) *abbreviated Title of Journal*, (3) **Volume Number** of Journal (Periodical), (3) issue number in year of publication, (4) the article's starting page number–final page number in Journal (Periodical), and (4) (Year of publication) (for example: O.V. Mikhailov, *Rev. Inorg. Chem.*, **30**, 4, 199–273 (2010)).

In Collection of Articles and **Books** (1) Initials and Surnames of all the authors given in the order appeared in the article in its original language, (2) In: *Title of Collected Volume (Book)*, (3) Publisher, (4) City, (5) Year of publication, and (6) cited page(s) (for example: G.I. Likhtenshtein, In: *Okislitel'no-vosstanovitel'nye metallofermenty i ikh modeli (Oxidation-Reduction Metalloenzymes and their Models)*, Part I, IKkF AN SSSR, Chernogolovka, 1982, pp. 7–10, 13, 16.).

1.2. For books and monographs:

When they are cited as a whole (1) Initials and Surnames of all the authors given in the order appeared in the book in its original language, (2) *Title*, (3) Publisher, (4) City, (5) year of publication, and (6) total number of pages (for example: D. Perrin, *Organicheskie analiticheskie reagenty (Organic Analytical Reagents)*, Mir, Moscow, 1967, 407 p.).

When only selected pages are cited (1) Initials and Surnames of all the authors in the order appeared in the book in its original language, (2) *Title*, (3) Publisher, (4) City, and (5) cited page numbers (for example: D. Perrin, *Organicheskie analiticheskie reagenty (Organic Analytical Reagents)*, Mir, Moscow, 1967, pp. 224–227.).

1.3. For inventions (1) Reduced form from the word 'Patent' or from 'Inventor's Certificate', (2) name of Country where the patent is issued, (3) Number of Patent or Inventor's Certificate, and (4) (year of issuing the patent) (for examples: Pat. USA 4.318.977 (1982); Inventor's Cert. USSR 1.340.410 (1987)).

1.4. For dissertations (1) Initials and Surname of the author, (2) Science Degree (Field of Science), (3) Name of Institution where the dissertation work is performed, (4) City where this institution is located, (5) year of publication, and (6) total number of pages (for example: T.N. Lomova, *Dr. Sci. (Chem.) Dissertation*, Institute of Chemistry of Non-Aqueous Solutions, USSR Academy of Sciences, Ivanovo, 1990, 456 p.).

For author's abstracts of dissertations (1) Initials and Surname of the author, (2) the word '*Extended Abstract*', (3) Science Degree (Field of Science), (4) Name of Institution where the dissertation work is performed, (5) City where this institution is located, (6) year of publication, and (7) total number of pages (for example: P.V. Gushchin, *Extended Abstracts of Cand. Sci (Chem.) Dissertation*, Saint-Petersburg State University, St.-Petersburg, 2010, 16 p.).

1.5. For meeting papers (1) Initials and Surname of all the authors in the order appeared in the collection of abstracts in its original language, (2) *Name of Conference, Symposium, or Congress*, (3) (*Translation of Name*), (3) (Place, Dates, Year), (4) Publisher (if indicated), (5) City, (6) year of publication, (7) book volume (if available), and (8) the abstracts's starting page number–final page number (for example: S.I. Dorovskikh, L.N. Zelenina, N.B. Morozova, and I.K. Igumenov, *XVIII International Conference on Chemical Thermodynamics in Russia* (Samara, Russia, October 3–7, 2011), Abstracts, Samara, 2011, Vol. 1, pp. 83–84.).