

RULES FOR AUTHORS

Basic provisions

The Journal "Butlerov Communications" presents scientific publishing interests of very specific scientific community – members of the Editorial Board, participants of the Scientific A.M. Butlerov Foundation (any researcher may become a participant of BSF), of researchers working in organizations that are co-founders of the journal (co-founders are required to subscribe to one set of annual journal and actively participate in the activities of the Scientific A.M. Butlerov Foundation) and other organizations, having an annual subscription to the journal. For researchers of this scientific community articles are published free and promptly (within 2 weeks), but in compliance with all peer-review standards!

Articles of other researchers who are not members of our scientific community are also accepted for publication free of charge, but they are handled after handling articles of researchers from our community, that is, they are not published promptly. We do not take fee for prompt peer-review in contrast to what is proposed by the State Commission for Academic Degrees and Titles in its latest recommendations!

Scientific direction of the periodical – all areas of knowledge related to chemistry. According to the subject heading code in elibrary.ru the scientific direction of the journal could be related to the following branches: Chemistry; Physics (in areas related to chemistry); Biology (in areas related to chemistry); Chemical technology; Artificial intelligence algorithms and programs (potentially relevant to chemistry).

The Journal "Butlerov Communications" is the official publishing organ of the Scientific A.M. Butlerov Foundation (<http://foundation.butlerov.com/>) and supports the co-sponsorship Institute. Composition and number of the co-founders of the journal change each year depending on readiness of universities and research organizations to provide real support to the journal and organizational support to the Scientific A.M. Butlerov Foundation. Unchanged co-founders of the journal are the Public Organization «D.I. Mendeleev Tatarstan Republican Chemical Society» and JSC "Innovative Publishing House "Butlerov Heritage". With other organizations the agreement on scientific and publishing cooperation is signed that fixes their status of the journal co-founders. A complete list of co-sponsoring organizations is presented on the official web portal of the journal (<http://butlerov.com/>).

Thematic areas of the Anglo-Russian Journal "Butlerov Communications" can be conventionally grouped under the following thematic headings:

Thematic Sections

- Agrochemical Research
- Biochemical Studies
- Geochemical Studies
- Investigation of artificial intelligence algorithms
- Research of dependencies "structure – property"
- Study of catalytic processes
- Research into new materials
- Study of Reactivity
- Study of the properties of substances and materials
- Study of the properties of catalysts
- Investigation of the physical phenomena
- Study of chemical reactions
- Quantum-chemical investigations
- Formulations Research
- Applied research
- Theoretical Studies
- Technological Studies
- Physico-chemical Studies
- Chromatographic Studies
- And others.

Thematic Subsections

- Biochemistry
- Kinetics and Catalysis
- Organometallic chemistry
- Inorganic Chemistry
- Organic Chemistry
- Industrial Chemistry
- Structural Chemistry
- Theoretical and Computational Chemistry
- Theory of Reactivity
- Toxicological Chemistry
- Physical chemistry of high temperature
- Physical Chemistry
- Chemistry of biologically active substances
- Chemistry of renewable vegetative resources
- Chemical Industry and Technology
- Chemical Physics
- Electrochemistry
- Organoelemental Chemistry
- Pharmacology
- and others.

However, the journal takes also publications and related fields of knowledge relevant to chemistry.

Author's material may be presented as:

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|---------------------------------|--|
| • Author's Review | • Review |
| • Analytical Review | • Letter to the Editor or responses from readers (1-2 pages) |
| • Information for discussion | • Full Paper |
| • Research Review | • Promotional Column |
| • Historical column | • Anniversary Dedication |
| • Brief Communication (3 pages) | |

It must be borne in mind that Promotional Column, Anniversary Dedication, as well as the materials not relevant to chemical profile of the journal will not be considered to be SAC publications!

Articles are published providing there are graphical abstract, as well as the English translation of the "headers" of articles, including the abstract and obligations of subsequent operational full-text translation into English of the final (we particularly emphasize it!) editorial version of your article.

The journal does not accept copies of posters of various conferences, or their analogues, similar in style of presentation, from individual authors, as these posts have very low data-intensive and high degree of uncertainty. However, the journal provides opportunity to publish (as a supplement to the issue) complete electronic copy of abstracts of conferences, as well as full-text reports of various chemically oriented conferences (in agreement with the organizers of the conference). Additionally, the report authors are provided the opportunity to publish this material in expanded form in English and Russian languages in the form of full publication. This material is recommended to be fully complemented with the extended introduction, specific data, techniques, detailed conclusions and so on. The author should get away from sketchy presentation of the material and bring it at least to the level of short messages or letters to the editor.

The journal is particularly convenient for the creation and preparation for printing of large and science intensive publications, monographs, books, since a part of work on the detailed systemization and design of the material takes place during editorial processing of a series of articles on the website pages of the journal.

The combination of possibilities declared here in conjunction with Internet portals of the journal and Scientific A.M. Butlerov Foundation, will enable authors to ultimately create versatile and valuable personalized, individual and collective information and scientific structures, including, in addition to the specific databases and knowledge, the reflection of personal views on the subject of study. This allows focusing on the corresponding field of knowledge not using the impersonal databases, but by a particular researcher verifying methodological approaches to solving certain classes of problems.

The principal advantages of our journal are the following possibilities:

- The journal generates editorial portfolio of articles submitted for publication as well as forum discussions of permanent online conferences. Accordingly, the subject matter of the journal is defined by the themes of these internet conferences and, when necessary, the internet-conferences may change their subjects or the new ones will appear.
- Support for the service of permanent (versioned) updating the electronic format for all published material (retaining the original source).
- The possibility for the authors to present this material on an unrestricted basis within reasonable limits.
- Maximum-operative publication of copyright material (subject to the editorial requirements).
- Feedback support of Editorial Board with authors.
- Possibility for inclusion of editorial references, comments, etc. into the author's material.
- Support of the reader's feedback opportunity (comments, notes, supplements and etc.) at forums of permanent Internet conferences, suggesting an editorial proofreading. It is possible for the author to answer the remarks and comments of the readers having scientific degrees. Moreover, those who participate in discussions at our forums are granted copyrights with fixing the date of contribution for scientific data corresponding to the novelty criteria.
- Opportunity to view the materials of the journal in online database mode.
- Author's material is promptly considered by the Editorial Board and visualized online as it becomes available in the current issue of the journal.

Provision on peer-reviewing of the journal "Butlerov Communications"

The purpose of the review is to ascertain the compliance of the article with scientific and editorial standards, to exclude methodological errors and falsifications.

The articles contributed to the Editorial Board of the journal are reviewed by the specialists with the scientific degree of the doctor of science in the specialty of scientific theme of the article. In some cases, additional review may be written by a candidate of sciences, subject to his high qualification. Reviewers give a reasoned opinion on the appropriateness of the article's publication.

The main requirement for the published material is its conformity to high scientific standards and criteria of novelty. Authors who publish their article for the first time in our journal should provide a review of Doctor of Science (reviewer from the author) to the article, since it is important for us to know that someone can vouch his name for the submitted author's material. For other authors, it is an urgent wish. However, the presence of positive reviews, provided by the author's reviewers, is not a sufficient reason for the publication of the article.

Review should be signed, stamped by the organization and contain full contact information about the reviewer (place of employment, position, phone, E-mail) for feedback from them. Only then we attract the full members of the Editorial Board to review the author's material. The reviewers may be either full members of the Editorial Board, or do not it. If the subject of the article is beyond the scope of competency of the members of Editorial Board, external reviewers, recognized specialists in a particular field of knowledge are attracted.

In the presence of 2 positive reviews, the article is published. Review may take the form of separate documents, or it may be summed up by the executive editor (for example, if the discussion of author's material was conducted by e-mail or on closed editorial forums on the page of the reviewer in the internet-portal of the journal) in the form of a review in the initial or revised editorial file of the article as editorial notes, if necessary, with appropriate revisions and comments in context, with marks in red. The final decision on accepting or rejecting the material (evaluated as a separate review by default) is made by the Chief Editor of the journal.

In cases of dispute, if the article is debatable, it can be published in the discussion section by the decision of the editor.

If the reviewer has criticism on the work demanding author's participation to dispose of ambiguous places, the article is sent to the author for correction. If the authors clearly considered all reviewers' comments and made the necessary changes or convincingly confirmed the rightness of their position in the text by making the appropriate explanations and reviewer agrees with revisions, the article is approved by the executive editor and the chief editor for publication. If the amended article does not satisfy the reviewer, the Executive Editor and / or the Chief Editor decide on attracting additional reviewers or rejecting the article.

Review, at the discretion of a reviewer or Executive Editor, can be conducted confidentially and has either closed character or with the open authorization of the reviewer. Reviews or editorial comments with indication of review authors can be provided on request of expert councils of Higher Attestation Commission of the Russian Ministry of Education.

Reviewer has the right to point out the need for additions and refinements to the manuscript, which is then sent to the author for revision.

Reviewer has the right to make recommendations to the author and Editorial Board to improve the manuscript. Reviewer's comments and suggestions should be objective, principle, and aimed at increasing the level of the manuscript.

Terms of reviewing in each case are determined by the Executive Editor with the maximally prompt publication of the article.

In the review, it is desirable to cover the following issues:

- compliance of the article content with the theme stated in its title, as well as the profile of the journal;
- relevance of the work;
- scientific novelty (originality in achieving the objectives of research);
- appropriateness of publishing the article with account for the coverage of the issue in the existing literature;
- logicity, consistency and coherence of presentation, логичность, последовательность и связность изложения материала, clearness of tables, diagrams, figures, correctness of formulas;
- evaluation of strictness and uniqueness of conclusions their adequacy to the main ideas of the article, theoretical and practical significance of the material;
- design quality (compliance with editorial requirements);
- Advantages and disadvantages of the article and recommended corrections and additions.

However, the reviewer may select from this recommendation list the most important characteristics for the particular case, provided that the rest does not cause problems. Reviewer gives a conclusion about the possibility of publishing the article, "recommended", "recommended after correcting drawbacks noted by the reviewer" or "not recommended."

All author materials are contributed to the editors through on-line procedure on the official site of the journal (<http://butlerov.com/>), in some cases, sending by email is possible (butlerov@mail.ru). All authors of the article or, at least, the leader of the thematic direction and corresponding author are required to undergo a full registration, reporting all necessary personal information about them. The process of reviewing the article is fully displayed on the website of the journal being available to all members of Editorial Board and authors of the particular article.

The activity of the journal is regulated by the relevant laws of the Russian Federation and the international community, so the authors of the Russian Federation should supplement the contributed material corresponding to the criterion of scientific novelty with the expert conclusion about the possibility of publication of author's material in the open press (possibly sent by E-mail, fax or regular mail). Authors from other countries should be guided by their own legislation. **Responsibility for the publication of confidential material rests entirely with the authors.**

Language

The journal "Butlerov Communications" is an English-Russian scientific edition, so the authors of articles published in Russian have to forward to us the full text English translations of their articles within 1 month (without this commitment, we do not publish articles!!), and the "headers" of the article, including abstract is contributed in English to the editors office simultaneously with the full-text Russian version. Without this commitment, we do not publish articles! Translations should be done from the final editorial Russian version of the article (but not from the initial or intermediate versions), which is downloaded from the journal site in Word format. Please comply with the accepted article formatting.

Please note that it is unrealistic for the Editorial Board to translate all the articles. If you do not perform your obligations, the journal would not be fully English and would not abruptly enhance its prestige and impact factor, which is important for all of you!

It should be borne in mind that neither the Editorial of the journal, nor Russian-speaking authors are native English speakers and, accordingly, we cannot guarantee that the English translation is impeccably correct. In this regard, on the website of the journal there will be initially visualized the author's English version of the article (if available) as a preprint, i.e. unreviewed message (regarding English spelling) with the output data, which coincide with the Russian version, but the pagination will contain the letter P and this will be written in the header section. Next to the number of such electronic journal issue of Butlerov Communications it will also be indicate that this issue is a peer-reviewed publication of the English-language preprint of the Russian version of the journal issue. However, since January 2014 International Editorial Board of the English version of the journal Butlerov Communications (with the participation of western scientists) starts its work. It will form from the available translated articles-preprints the issues of the © *Butlerov Communications*. 2015. _____ Kazan. The Republic of Tatarstan. Russia.

international publications with verified English language context, peer-reviewed by native English speakers. Not all articles of the journal Butlerov Communications will get into the English language version. Moreover, articles from different numbers of the Russian version will again be configured by topics, might be extended, partly changed or, on the contrary, reduced at the request of international councils of the journal Butlerov Communications and reviewers, and subsequently new output data will be assigned to the articles in both electronic and printed editions of the journal. English-speaking authors will be able to send the article directly to Butlerov Communications, whereas the Russian-speaking authors shall first be published in the Russian version of the journal "Butlerov Communications".

Recommended structure of publication

The authors' material should be contributed in the format **.doc** of the text editor Word. It is desirable to use as a layout constant the examples of articles from the site. In using E-mail, При использовании электронной почты, it is recommended to back up the file using zip-archiver. The total file size should be not more than 10 Mb. With a larger size the material should be divided into several smaller files.

The volume of material presented is not limited (within reason) and we welcome the most complete descriptions, details, definitions, predictions and conclusions. Still the publication should be whenever possible divided into chapters and sub-chapters with common titles, each optimally not exceeding 8 printed pages of A4. The latter greatly facilitates the perception of on-screen text, but is not strictly necessary. For all chapters it is desirable to have overall, sequentially numbered literary references, compound numbers, tables, figures and so on.

Submitted material must contain the following information:

- If the authors open or continue Thematic Course, it is necessary to submit the name of the direction and the serial number (for example, Part IV). Indicate where the previous message was published.
- Title of the publication
- Surname, first name and patronymic.
- Name of the organizations where the work is done. The mailing address of the organization, including the name of the department.
- Telephone, fax, E-mail and Internet address for each organization or authors.
- Through an asterisk (*) indicate authors – leaders of the direction.
- Through a symbol (+) indicate who will support the ongoing correspondence with the editors and will support subsequent updates (other authors may also contact the Editorial).
- Keywords.
- Abstract providing basic information about the purpose and subject of study, the main findings and conclusions. One-sentence abstracts are not accepted!
- Graphical abstract as a generalizing scheme or figure, for example, the main reaction (source product), the structure of the investigated compounds, photographs or graphics, etc., containing brief explanations.
- The following sections are desirable:
 - Introduction
 - Results and Discussion
 - Chapters and subchapters
 - Experimental
 - Conclusions
 - Acknowledgements
 - References and etc.

Authors must adhere to the International System of Units (SI) and the rules recommended by the international organization of IUPAC. All abbreviations (except for some common, such as the X-Ray data) are decrypted at the first appearance in the text. In the case of a large number of abbreviations their decrypting is provided in a separate list. The number of significant figures in the tables should correspond to the actual errors of measurements or calculations.

Style of the submitted material is not strictly regulated, but must meet the general requirements of the leading scientific periodicals. For example, it is acceptable for surveys to keep to the style, worked out in *Chemical Review*, for research publications – *J.Am.Chem.Soc.*, etc.

Editorial strongly recommends the authors already now attach their material with corresponding geometries of basic molecules and transition states (in files) obtained by calculation methods (with full comment), and we recommend to accompany X-ray analyses with CIF-files of crystalline structures which would be submitted in the Intellectual System of depositing scientific and scientific-technical data (ISD), being currently developed by A.M. Butlerov Scientific Foundation. With the introduction of ISD in full form, authors will be able to deposit (i.e., get the output data for the block of scientific information) information and other relevant research data (such as the physical characteristics of the new compounds, methods of synthesis, etc.), including those which have not yet been published in articles

Supporting information

All authors of the publication, or at least, the leaders of thematic direction and correspondence supporters are required to undergo a full registration on the website of the journal, giving all necessary personal information about themselves in Russian (for Russian authors) and in English (from the time of full operation of the English version of the journal). Information about each author should include the following items:

- Surname, first name and patronymic;
- Photography (portrait, desirable qualitative, color, free style) in the format **.jpg**;

- Brief biography or detailed scientific becoming;
- Workplace;
- Position;
- Office number;
- Home and cell phone (available only to the Executive Editor and needed for operative communication),
- Fax,
- Personal E-mail;
- PhD;
- Position;
- Research interests.

It is also recommended to inform about:

- Area of educational activities;
- Selected list of scientific papers (at the discretion of the author). It can accommodate full-text copies of publications;
- Advertising own scientific developments and achievements;
- The optional photo (free style, desirably qualitative, color) in the format **.jpg**;

It is possible to present at additional information that should be reflected in the Internet (supervision of graduate students, description of the creative team, etc.).

Authors' obligations

The author of the article published in Russian still retain the obligation to redirect to us the full text English translation of the final editorial version of the article (we specially emphasize that not the source or intermediate author's material) within 1 month, wherein the "headers" of the articles, including the abstract, are contributed to the Editorial Board in English at the same time as the full text Russian version. Without this commitment, we do not publish articles!

Each article published in the journal is classified by categories and placed for discussion on a specially created Web forum in the relevant thematic permanent Internet conference of the journal. That is why the **publication in the journal automatically imposes an obligation on the authors to participate in scientific debate based on their publication in our Web-forum of the Internet conference and the need to constantly update the material presented, by adding new information on their own results and the latest published data**. Due to the fact that the published material is constantly updated on Web-forum by the ideas and information of the participants, and all the discussion material is periodically subjected to editorializing, and the authors themselves or on editorial request are obliged to provide the rapid provision of additional information available to them (e.g., conditions and methods of synthesis of compounds, their properties, quantum-chemical and X-ray data, various descriptions, comments, statements and so on). The supplement to the publication thus formed will always accompany it in the electronic versions of the journal and republished in print indicating the newly-formed output data, such as:

Sidorov S.S., Petrov P.P. *Supplement on discussion materials from the online conference "Butlerov Readings" to the article*: Uryadov V.G., Ofitserov E.N. Nature of the transition state of cycloaddition in the liquid phase. Part I. On the elementary motion of the molecules in the liquid. *Butlerov Communications*. **2005**. Vol.6. No.1. P.1-12 (supplement P.13d-15d).

Part of such additional information provided will be integrated into the collective, personal, personalized, and other public and private databases and knowledge bases. For the parties to the scientific debate on Web-forums webcasts of the journal, secured copyrights for the entire discussion paper matched the criteria of novelty and fixed the date of receipt. Copyrights are secured for all discussion material corresponding the criteria of novelty with the fixation of the data of receipt over the participants of scientific discussion on Web-forums of internet-conferences of the journal,

Attention! Responsibility for publishing the information not to be published in the open press on the Web-forum lies entirely on the particular participant of debate. For the discussion material, requiring expert conclusion, this conclusion should be simultaneously sent to participants of the discussion by email (*E-mail: butlerov@mail.ru*), or it can be done on the request of the Editorial Board later. In the event of legal collisions, the Editorial Board of the journal is entitled to remove from the electronic and printed versions of the journal problematic materials and change the output data of the Supplement to the paper.

Instructions for the preparation of the publication

Text in the Format **.doc** of the text editor Word should be

- typed by font TimesNewRoman (preferably 12pt); special symbols – font Symbol; text for figures, schemes and tables, as well as the text of abstract should be typed with the use of the font size 11pt;
- with single-spaced interval;
- typed without hyphenation and using points to indicate fractional numbers (for example: 12.87);
- checked for spelling errors using the service WORD "spelling".

Captions for tables and charts should precede the latter. Captions for figures should be under them. Tables and Figures should be cited in the text (for example, Fig. 1; Tab. 1). Figures and photographs should be very clear (possibly

colored, but without losing the semantic filling when transferred into black and white mode) and presented in the format **.tif** or **.jpg**. It is desirable that the figures and tables were as compact as possible, but without sacrificing quality.

To create mathematical formulas you should use formula editor Microsoft Equation, but maximize the opportunities of fonts TimesNewRoman and Symbol. When preparing the chemical formulas and chemical reaction schemes, it is necessary to use special chemical editors, such as ChemWindow, ChemDraw, ISIS/Draw (it is optimal to use the program ChemOffice, version 6.0 and higher) and so on, or to present the formula drawings in the format **.tif** or **.jpg**, necessarily after checking the quality of their printed version.

References in the paper are given as the numbers in square brackets.