*Chemistry of Heterocyclic Compounds* **2016**, *52*(12), 1093–1097

# Instructions to authors

## 1. General statement

1.1. The international journal "Chemistry of Heterocyclic Compounds" ("Khimiya Geterotsiklicheskikh Soedinenii") publishes original papers, reviews, minireviews, microreviews (section "Heterocycles in Focus"), and short communications dealing with the chemistry of heterocyclic compounds in Russian (free-access on the journal's website – hgs.osi.lv) and in English. The Journal also publishes reviews and annotations on new books as well as brief reports on conferences in the field of heterocyclic chemistry, commemoratives dedicated to prominent chemists in the field of heterocyclic chemistry.

The author is fully responsible for the reliability of experimental data presented in his/her paper.

1.2. **Original papers** should present timely, complete, rigorous, previously unpublished research of experimental and theoretical scope that would be of interest to a diverse readership. The paper may concern synthesis, structure, reactions of heterocyclic compounds or their direct precursors, as well as their biological activity, physicochemical and other properties in the context of their synthesis. Transformations of substituents in a heterocycle may be considered when their character is specific, due to a special effect of the heterocyclic system. Research based on analogy (trivial replacement of substituents or change of reaction conditions) without demonstration of its specials importance will not be considered. Original papers ought not exceed 15 journal pages.

1.3. **Short communication** should contain substantially new results or methods of general applicability or interest, or focused studies requiring the claim of precedence. Only those experimental data and literature references necessary for confirmation of the main conclusion should be presented. The synthesis of known compounds by a new method should be illustrated with at least 5 examples. Short communications should not exceed 4 journal pages.

1.4. The topic of a **review or minireview** should be submitted for preliminary approval by the Editors in the form of a detailed (1-2 pages) summary containing information regarding the main parts of the paper, the time frame of the literature reviewed, and previous reviews on that topic. The thematic of microreview ("Heterocycles in Focus") also has to be approved prior to submission.

Reviews should be comprehensive, critical, and readable accounts of the newest research in heterocyclic chemistry. The reviews or minireviews should cover the topics that present sufficiently general interest for heterocyclic chemistry or reflect an important aspect of practical application of heterocyclic compounds in industry, agriculture, medicine, etc. Microreviews ("Heterocycles in Focus") represent a compact compilation of recent (last 5–10 years) information on a selected heterocycle: its synthesis, properties, or applications as a product, reactant or ligand; or starting materials or reagents for the synthesis of heterocycles. Only the most important information is given showing the main advantage of the method in one-two sentences. If possible mechanisms and intermediates should be omitted in schemes, but they can be discussed or named in the text.

The time period and the scope of the subject area should be clearly defined in the introduction. Review manuscripts should not exceed 25 journal pages, minireviews – 6 pages, microreviews ("Heterocycles in Focus") – 3 pages.

## 2. Manuscript evaluation and acceptance

Only submissions prepared according to the Instructions to Authors will be considered. The preliminary evaluation of manuscripts as to their fitting into the scope of the journal, their originality, and their timeliness will be carried out by a section editor. All manuscripts in compliance with the journal's requirements will be reviewed by two or more referees. The decision regarding microreviews ("Heterocycles in Focus") can be taken on the basis of one referee's recommendation. Authors are invited to suggest at least 3 potential referees with no conflict of interest. Referees evaluate manuscripts on their significance, scientific rigor, originality, degree of interest to the heterocyclic chemistry community, thoroughness of compound characterization, appropriateness of the cited literature, and quality of writing.

The evaluation process is confidential. An exception is possible only in the case when a referee alleges an intentional presentation of falsified data in the manuscript. The referees are asked in their reports to indicate the aspects of the paper under review that make it interesting for the journal's readership, as well as deficiencies in the presented results that would not allow for the paper to be published.

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The section editor makes the final decision about the acceptance of the submitted manuscript for publication in the Journal.

At the time the manuscript is submitted to the Journal, and during its evaluation, no other manuscript reporting the same results may be submitted to another journal.

### 3. Manuscript organization

The manuscript should be concisely written, thoroughly drawn up, and carefully edited by the authors. It should be easy to understand and the results should be reproducible.

3.1. The text of the manuscript must begin with the **title**, which should attract the reader's attention fully and correctly disclose the essence of the work at the same time being concise and clear. It is desirable to mention in the title the principal heterocyclic system treated in the article. Abbreviations should be avoided. When a publication is a serial communication, a footnote should be added (to the number of communication) referring to the preceding paper. Serial communications are numbered with Arabic numerals (e.g., for communication 8, see[1]).

3.2. The title of the paper should be followed by the **authors full names**. The name of the corresponding author (s) should be marked with an asterisk (*). After the name of each author, the institutional affiliation should be marked by a roman numeral in superscript (example: Alexander S. Alekseyev[1]*, Gennady I. Popov[2], Inna V. Ivanova[1]).

3.3. Next full **name(s) of the institution(s)** where the work was performed and the location(s) (including street address or P.O. box number, city, postal code, and country) should be provided. Each address line should be followed by the **e-mail address** of the author representing the institution.

3.4. **Abstract** should start with a graphical representation of the results in the form of a structure or reaction equation which in connection with the title should attract the readers' attention and give a representation of the article's content. The graphical part of the abstract should be followed by a brief text where the purpose of the research, the main results, and the major conclusions of the study should be stated. The abstract should not contain codes of the compounds, abbreviations, experimental details, or reference citation numbers.

3.5. **Keywords** should then be given (5-10) reflecting the general type of the compounds under investigation and the character of the reactions. If, in the opinion of authors, the number of keywords necessary to adequately describe the presented research is higher, they may choose to leave out those terms already present in the title or abstract of the paper.

3.6. In the initial paragraph of the **main text** a brief discussion of the available literature on the present research topic should be given, and the importance of the topic with respect to the interests of the readership should be indicated. The deficiencies of known methods should be pointed out, and the possibilities created by a successful solution to the problem should be presented. The purpose and objectives of the research done by the authors should be clearly explained. The methods that could be employed to achieve them – those known from literature as well as alternatives – should be analyzed. Afterwards, the results should be presented and explained, details of the syntheses analyzed, and the possible limitations demonstrated and discussed. Only those spectral data, which are essential for confirming the structure of the synthesized compounds should be mentioned and discussed. Duplication of the same data in text, tables, and figures should be avoided. For new synthetic methods, a discussion of the reaction mechanism is desirable. The main text ends with a brief conclusions section about the performed research that does not repeat the abstract.

3.7. At the beginning of the **experimental** section, the instruments that were used to characterize the synthesized compounds should be named. The sources of all non-trivial reagents used, their commercial source or literature references for their synthesis should be given. Each paragraph describing a synthetic experiment should start with the product's systematic (IUPAC) name and the structure number assigned to the compound in the discussion section. For all new compounds, evidence adequate to establish both the identity and degree of purity (homogeneity) must be provided. In particular, the elemental analysis results or high-resolution mass spectral data should be provided, as well as $^{1}$H and $^{13}$C NMR spectra. For the known compounds synthesized following a published procedure, a reference should be given. For the known compounds synthesized by a new or modified procedure, physical characteristics and spectral data used to confirm the identity of the structure should be given together with the method of synthesis and a reference to the literature data. Section 4.6., 4.7., and 4.8. should be used for guidance on reporting the experimental procedure and compound characterization as well as spectroscopic, crystallographic, and computational data.

If, in the opinion of the referees or the Editor, new compounds have not been satisfactorily characterized, the paper will not be accepted. The Editor may accept a submission, which does not contain all the required characteristics of the new compounds if, in his/her opinion, the presented data are sufficient to prove the structure of the compounds.

3.8. The main text of the paper should end with a **list of references**. The references should be numbered with Arabic numerals in the order of their appearance in the text, and the corresponding citation numbers should be inserted at the appropriate locations in the text in superscript. In the list of references, it is permitted to combine several related references under a single number. The conventional abbreviations for the titles of journals and handbooks should correspond to those used in *Chemical Abstracts*. References to unpublished results or private communications may be given only as footnotes; they should not be numbered or included in the reference list. The only exceptions are papers by the authors, previously submitted to *Chemistry of Heterocyclic Compounds* (*Khimiya Geterotsiklicheskikh Soedinenii*), but not yet published. These may be included in the reference list with the full title of

the paper mentioned. References to internet resources should be presented in a format that facilitates their easy access.

3.10. The authors are invited to submit supplementary materials (in English), that are not included in the article's text, for example, graphics of the spectra or figures combined into a *doc* file, as well as *fid*, *cif* or other files. For microreviews ("Heterocycles in Focus") files of author's photos have to be submitted as separate *jpg* (300 dpi) files. The graphical abstract should be uploaded as a supplementary file.

## 4. Manuscript presentation requirements

4.1. Manuscripts must be prepared using *MS Word* as *doc* or *docx* files. To properly format the manuscript, the template from the journal's website (http://hgs.osi.lv/index.php/hgs/about/submissions) should be used. Equations, schemes, tables, and figures must be placed within the main text after being first mentioned there and numbered strictly in the order of their mentioning. All tables should have a title and all figures should be supplied with captions that do not duplicate the main text; reaction schemes may have captions if necessary. The variables or physical characteristics given in the column titles of tables should have measurement units added after comma (for example "Yield, %").

4.2. Common abbreviations, acronyms, and symbols may be used, but less common ones should be defined the first time they are used.

The dimension of the units is given in accordance with the International System of Units. The symbols used for physical constants should be in italics (e.g., *d, J, k, c, m/z*), but the respective units of measurement should not be italicized. Abbreviations of words *secondary* and *tertiary*, as well as abbreviations of prefixes *ortho*-, *meta*-, *para*-., etc., should be written in formulas with italicized Latin alphabet letters like *s*-, *t*-, *o*-, *m*-, *p*-, *i*-, *cis*-, *trans*-.

4.3. Chemical **structures** should be written using *ISIS Draw* (*Symyx Draw*) or *ChemDraw*: font *Arial*, size 8 pt, bond length 0.41 cm (or as ACS document 1996 styled and reduced to 80%). The scheme width should not exceed 17.5 cm (two column arrangement) or 8.5 cm (one column arrangement). Graphical abstract width not more as 9.5 cm, high – not more as 4.5 cm. All of the reaction conditions should be indicated above (reagents, catalysts, solvents) or below (temperature, time) the reaction arrow. If the indications of conditions make the scheme excessively crowded they can be placed at bottom of the scheme marked with letters i, ii, etc., for example "*i*: HCl, $H_2O$, 80 °C, 5 h". The same letter should be placed above the corresponding reaction arrow. All words and abbreviations in schemes have to be written in English.

4.4. The **figures** must be submitted as separate files in *jpg* format with a minimum resolution of 300 dpi, the dimensions should not exceed 8.5 cm. The size of a figure should allow one to see it in detail. Whenever possible, use numbers to identify items in a figure, and give the corresponding explanation of these numbers in the figure caption.

4.5. It is desirable to use standard abbreviations and unequivocal molecular formulas for reagents and solvents, as well as Arabic numerals for the reactants, intermediates, and products in the order of their appearance in the text. Compounds with related structures may use a common number, e. g., "RX (**2**)"; for their derivatives with different substituents, a letter is added to the number, e.g., "alcohol X = OH (**2a**), acetate X = OAc (**2b**), tosylate = OTs (**2c**)." When the full name of a compound is mentioned its numerical designation should be given in parentheses. Codes without a generalizing word should not be used, e.g., "the reaction of compound **2d** with amide **3**" – not "the reaction of **2d** with **3**". Stereochemical and structural symbols, characterizing structural peculiarities or a substituent position in a molecule, should be composed in italics, e.g., "(*R*)-enantiomer," "*tert*-butyl," "*p*-xylene", "*N*-alkyl", "pyridin-2(1*H*)-one". Cumbersome names of simple compounds should be replaced by their chemical formulas, e.g., "NaBr, TsOH" instead of "sodium bromide, toluenesulfonic acid".

4.6. The **experimental** section should be written in the past tense ("was boiled", "precipitated", etc.). The quantities of reactants and reagents should be given in both mass and molar units, e.g., "2-ethynylpyridine (0.103 g, 1.0 mmol)". The integer and fractional parts of a number should be separated by a decimal point. Yields should represent weighed amounts of isolated and purified products, and should be reported as mass and as percentage of the theoretical value. Preferably, integer numbers should be used, e.g., "Yield 93 mg (78%)" instead of "Yield 0.093 g (78%)". In molecular formulas, elements should be arranged according to the *Chemical Abstracts* system: C, H, and then all other elements in Latin alphabetical order. Formulas of molecular adducts and onium salts are given with raised dots, e.g. "$C_6H_{12}N_2 \cdot 2HCl$". When flash or thin-layer chromatography is used, both the stationary phase and eluting solvent should be identified.

4.7. The data characterizing the synthesized compounds should be presented in the following order.

**Melting and boiling point**. A melting point range and the appearance should be reported for every crystalline solid product, together with the solvent from which it was recrystallized (and literature data for known compounds), e.g., "yellow needles, mp 76–78°C (EtOH) (mp 77–80°C (*i*-PrOH)[12])". Similarly for liquids the boiling point and the look, e.g., "colorless oil, bp 127–128°C (10 mmHg)".

**IR and UV spectra**. The experimental section should contain the frequencies of the characteristic absorption band maxima, their extinction coefficients or logarithms thereof (for UV spectra), as well as the conditions under which the spectra were registered.

IR spectrum (thin layer), n, $cm^{-1}$: 1650 (C=N), 3200–3440 (O–H).

UV spectrum (EtOH), $l_{max}$ (lg e): 242 (4.55), 380 (4.22).

**$^1$H and $^{13}$C NMR spectra**. The solvent, instrument frequency, and the standard should be identified. If a standard other than TMS is used, its chemical shift on the δ scale should be given. To indicate the positions of protons, the designations of the type H-3, H-2,6 (for aromatic

protons) and 3-CH, 4,5-$CH_2$ (for aliphatic protons) should be used. Protons in complex groups, to which a signal relates, should be underlined below, e.g., "3.17–3.55 (4H, m, $N(C\underline{H}_2CH_3)_2$)". Substituents should be indicated as follows: 3-$CH_3$; the positions of atoms should be indicated as follows: C-3, N-4, etc. If a signal in the spectrum is described as doublet, triplet, etc. (rather than a singlet or a multiplet), it is necessary to present the corresponding value of spin-spin coupling constants (e.g., $^3J_{5,6}$ or $J_{CF}$). If additional investigations have been made in order to establish atom connectivities and spatial relationships, the 2D methods used should be identified. The $^{13}C$ signal assignments to individual atoms are accepted only on the basis of 2D experiments.

$^1H$ NMR spectrum (400 MHz, $CDCl_3$), δ, ppm (*J*, Hz): 0.97 (3H, t, *J* = 7.0, $CH_3$); 3.91 (2H, q, *J* = 7.0, $COOCH_2$); 4.46 (2H, d, *J* = 6.1, $NCH_2$); 7.10–7.55 (9H, m, H-6,7,8, $N\underline{H}CH_2C_6\underline{H}_5$); 7.80 (1H, s, H Ar); 7.97 (1H, s, H-5'); 8.13 (1H, dd, *J* = 8.2, *J* = 2.3, H-5); 11.13 (1H, s, NH).

$^{13}C$ NMR spectrum (125 MHz, DMSO-$d_6$), δ, ppm: 36.3 ($CH_2CH_3$); 48.5 (C-5); 62.3 ($CH_2CH_3$); 123.0 (C Ar); 125.8 (d, $^2J_{CF}$ = 26.1, C-3',5' Ar); 128.9 (C Ph); 134.4 (C-5a); 168.3 (C=O).

**Mass spectra** should be presented as numerical *m*/*z* and relative ion current values. The ionization method used, ionization energy, mass numbers of characteristic ions, chemical origin of these ions (if possible), and the intensity with respect to the major ion should be given. For chemical ionization, the reactant gas should be indicated. For the high-resolution mass spectra, if the experimental value is not that of the molecular ion the brutto formula and calculated value of *m*/*z* should be given for this ion.

Mass spectrum (EI, 70 eV), *m*/*z* ($I_{rel}$, %): 386 $[M]^+$ (36), 368 $[M–H_2O]^+$ (100), 353 $[M–H_2O–CH_3]^+$ (23).

Mass spectrum (CI, 200 eV), *m*/*z* ($I_{rel}$, %): 387 $[M+H]^+$ (100), 369 $[M+H–H_2O]^+$ (23).

**High-resolution mass spectrum**.

Found, *m*/*z*: 292.1684 $[M]^+$. $C_{17}H_{24}O_4$. Calculated, *m*/*z*: 292.1675.

Found, *m*/*z*: 335.0377 $[M+Na]^+$. $C_{13}H_{17}BrN_2NaO_2$. Calculated, *m*/*z*: 335.0371.

**Elemental analysis**.

Found, %: C 55.22; H 4.09; Br 20.42; Cl 9.04; N 7.18. $C_{18}H_{16}BrClN_2O$. Calculated, %: C 55.19; H 4.12; Br 20.40; Cl 9.05; N 7.15.

4.8. The **data of X-ray structural analysis** should be presented as a molecule chart (figure) with numbered atoms, e.g., C(1), N(3) (if possible, with thermal vibration ellipsoids). The Journal will not publish full crystallographic data, tables of atomic coordinates, or temperature factors. Instead, they should be deposited at the *Cambridge Crystallographic Data Center* (*CCDC*) (the deposit number should be indicated in the article) or submitted in the file of supplementary information.

4.9. The list of **references** should include the last names and first initials of all authors ("et al." is not allowed). References in languages not using the Latin alphabet should be given in transliteration. The titles of periodicals should be transcribed as in *Chemical Abstracts*. The reference section should be written as follows:

***Books***. The page or chapter should be indicated when discussing particular topics.

Pozharskii, A. F. *Theoretical Fundamentals of the Chemistry of Heterocyclic Compounds* [in Russian]; Khimiya: Moscow, 1985.

*General Organic Chemistry*; Barton, D.; Ollis U. D., Eds.; [Russian translation], Khimiya: Moscow, 1985, Vol. 9, p.45.

Katritzky, A. R.; Pozharskii, A. F. *Handbook of Heterocyclic Chemistry*; Pergamon: Amsterdam, etc., 2000.

***Papers in Collections and Handbooks***

Gulevskaya, A. V.; Pozharskii, A. F. In *Advances in Heterocyclic Chemistry*, Katritzky, A. R., Ed.; Elsevier: New York, 2007, vol. 93, p. 57.

Hulme, C. In *Multicomponent Reactions*, Zhu, J.; Bienaymé, H., Eds.; Wiley-VCH: Weinheim, 2005, p. 311.

***Journals***. Only for journals in which each issue begins with page 1 should the issue number be included. When citing an article from a journal translated into English, first the reference to the English version should be given, then, in square brackets, the reference to the original.

Uchuskin, M. G.; Makarov, A. S.; Butin, A. V. *Chem. Heterocycl. Compd.* **2014**, *50*, 791. [*Khim. Geterotsikl. Soedin.* **2014**, 860.]

On polycojugated structures see: (a) Wang, C.; Dong, H.; Hu, W.; Liu, Y.; Zhu, D. *Chem. Rev.* **2012**, *112*, 2208. (b) Anthony, J. E. *Angew. Chem., Int. Ed*. **2008**, *47*, 452. (c) Thompson, B. C.; Fréchet, J. M. J. *Angew. Chem., Int. Ed*. **2008**, *47*, 58.

Lukevics, E; Erchak, N. P.; Demicheva, L. E. *Khim.-Farm. Zh.* **1992**, *26*(1), 45.

Kahveci, B.; Menteşe, E.; Özil, M.; Ülker, S.; Ertürk, M. *Monatsh. Chem*. DOI: 10.1007/s00706-012-0916-0.

Sato, T. *Yakugaku Zasshi* **1957**, *77*, 771; *Chem. Abstr*. **1957**, *51*, 17941.

***Author Inventor's Certificates, Patents***.

Nasakin, O. E.; Nikolaev, E. G. USSR Author's Certif. 1168554; *Byul. Izobret*., **1985**, No. 27, 90 (in Russian).

Slade, R.; Klimova, Y.; Halter, R. J.; Yungai, A. J.; Weiner, W. S.; Walton, R. J.; Willardsen, J. A.; Anderson, M. B.; Zavitz, K. US Patent 2008249135.

Dunbar, J. E.; Zemba, J. W. US Patent 4764608; *Chem. Abstr*. **1994**, *100*, 14852.

***Theses***

Maiboroda, D. A. Abstract of Diss. Cand. Sci. (Chem.), Moscow, 1998.

Rodinovskaya, L. A. Theses Dr. Sci. (Chem.), Moscow, 1994.

Brines, J. L. Ph. D. Thesis, Rockefeller University, New York, 1989.

For theses, the URL may be listed, if available.

**Manuscripts that do not follow the above rules will not be considered for acceptance.**

## 5. The publishing process

Manuscripts for publication should be uploaded to the on-line submission system on the journal's web site

**http://hgs.osi.lv**

In order to be able to do this, the author must register there as a user (check the role "Author"). After the logging into the system, one should go to the hyperlink ["New Submission"] on the page "USER HOME" and then follow the instructions on the site. It is important to choose the correct section (Original article, Review article, Heterocycles in Focus, Short communications) and to enter the names of **all** co-authors.

The authors are asked to send to the Editorial Office a signed Consent to Publish by mail. A scanned copy of it should be uploaded as a supplementary file onto the on-line submission system. The Consent to Publish form can be found on the journal's website. When the paper is published, the copyright is transferred to the Publisher.

The author can follow the review and editing process from his/her user page on journal's website. Manuscripts retained for correction for more than one month or those requiring another revision will be considered as new manuscripts. In the case of delay of receipt of the proof from the author, the Editors reserve the right to publish the paper without the author's corrections. If the author does not return the galley proofs, the Editorial Office may publish the article without author's corrections.

Submission of manuscripts that are already published or under consideration in other journals is not acceptable.

Information concerning the journal *Khimiya Geterotsiklicheskikh Soedinenii* and its English version *Chemistry of Heterocyclic Compounds*, Contents of the journal issues, as well as Instructions to Authors may be found on-line:

**http://hgs.osi.lv**
**http://www.springer.com/chemistry/organic/journal/10593**

The manuscripts submitted after January 1, 2017, onwards should comply with these updated Instructions.

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