RULES FOR AUTHORS

Contributions should be sent to the Editorial Board of the Russian language Journal (not Springer), at the following address:

Editorial Board of Journal of Structural Chemistry
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1. The Journal of Structural Chemistry publishes, in Russian and English, original, theoretical and experimental research papers providing insight into the structural aspects of chemistry. The papers are divided among the following general sections: The theory of molecular structure and chemical bond; The study of molecular structure by physical methods; The structure of amorphous materials, liquids and solutions; The dynamics of structural transformations; Crystal structures; Supramolecular and nanodimensional systems; The structure of surface; Methodological and technical aspects of the experiment; Reviews; Short communications; Personalia. The journal will not publish engineering or polemical papers.

2. Manuscripts should be submitted to the Editorial Office of the journal by electronic mail and, if requested, by regular mail. The following information about the corresponding author should also be presented: full name, institution, position, complete address, electronic address (e-mail address to be placed in a footnote in the paper), phone and fax numbers.

All manuscripts should be submitted to the following address: jsc@che.nsk.su; Journal of Structural Chemistry, Institute of Inorganic Chemistry, Acad. Lavrent'ev Av., 3, 630090 Novosibirsk, Russian Federation.

3. Submitted manuscripts will be subject of peer review to assess scientific value of the contribution, its compliance with the journal profile and these rules. The decision on the suitability of a manuscript for publication will be made by the Editorial Board and will take into account the recommendations from the reviewers. Immediate acceptance, minor revisions or a major revision will be suggested.

4. The text of the manuscript should be typed in Microsoft Word, 1.5 spaced, using Times New Roman font, 12 pt size. Each Table or Figure must be mentioned in the text; their approximate positioning in the paper should be indicated.

5. The manuscripts will be of the following three types: Full Paper; Short Communication; Review Paper. Full Paper should clearly describe the results of studies on an up-to-date fundamental scientific problem and should contain scientific novelty. The size of Full Paper should not exceed 10 journal pages including Figures and Tables. Short Communications is a short, not more than four pages, paper reporting novel results without detailed description of the experimental procedures. Review Paper should not exceed 50 pages and should provide insight into the state of research in one of areas of structural chemistry and should include unbiased critical analysis of the literature covering the field.

6. Each manuscript should have a title, authors' names, full name(s) of the institution(s) where the research was conducted, abstract clearly and concisely mentioning the results, and up to 10 keywords. The main body of the manuscript should be divided into sections. The names of main sections may vary but most often will include Introduction, Experimental, Results and Discussion, and Conclusions. The list of references is to be given at the end. When necessary, the authors will add List of Abbreviations (after keywords), Acknowledgement(s) (before References) or other sections.

In addition to their manuscript, the authors should submit a Graphics for the Table of Contents (colored graphics is preferred), such as a Figure, Scheme or formula.

The authors should follow the International System of Units (SI units) and IUPAC recommendations. All short forms and abbreviations (except for common ones, such as XRD) are explained upon first appearance in the text. When a great number of short forms and abbreviations is used, they have to be listed in a separate section.
Each Table of numerical data should be accompanied with a number (Arabic numeral) and title. Table headings should indicate parameters' names and units. The absence of data is indicated with a dash. The Table may be accompanied with footnotes and comments.

The illustrations (Figures and Schemes) should be sharply defined, with figures and symbols of sufficient size. Figures should not be overwhelmed with notations and unnecessary details; the notations could be replaced with numerical or literal designations explained either in the caption or in the text. Figures should be either inserted in the Word file of the manuscript or attached as separate files. The following files are accepted (in order of decreasing preference): cdr, doc, pcx, bmp, jpg, gif, tif. Paper copies of illustrations (or photographs) should have a notation on their reverse side with Figure number, authors' names and paper's title. Figure captions should be provided on a separate sheet of paper.

References should be numbered in the order of their mentioning in the text, with the numbers indicated in the text in square brackets, and listed at the end. Below examples of correct referencing are given:


**Program:** Sheldrich G.M. SHELX-97, release 97-2. – Germany, University of Goettingen, 1998.


While referencing papers in journals that have translated editions, both original and translated versions may be given.

7. *Introduction* should shortly review the current state of the field in which the study was accomplished (citing related work reported by other authors, including very recent work, is highly desirable), state the purpose of the study and justify its urgency and fundamental significance. *Experimental* section should describe used materials, methods of measurement, instrument specifications, programs and methodology. While reporting and discussing results (*Results and Discussion*), it should be made clear which results were derived in the present study, which facts were taken from other work (this work should be cited) and which statements were introduced by the authors in form of postulates, hypotheses or conclusions.

The manuscripts should not present excessively detailed description of experiments, syntheses and methodological approaches, long Tables of numerical, spectroscopic or crystallographic data (for instructions on the preparation of papers reporting crystal structures see Supplementary). Figures and Tables preferably should be combined in order to reduce their number (for instance, one Figure showing several spectra instead of several Figures; one longer Table instead of several short Tables). The Editors of the journal keep right to introduce minor reductions and changes in the manuscript.

8. Proofs will be passed to the authors directly, by electronic or regular mail (using contact information given in the manuscript). Authors should submit their corrections to the Editorial Office within 48 hours. Changes and additions to the text and Figures may be accepted only in exceptional cases.

9. Once paper published, the authors will receive either hard (10 reprints) or electronic (as a file) copies of the paper.


    Citing a paper published in the original and English versions of the journal:


11. The journal is surveyed by leading abstract services and databases: Chemical Abstracts, Chemical Titles, Current Contents, Web of Science and others.
Supplementary: Format for papers reporting crystal structures

Due to growing number of crystal structures and increasing role of electronic resources, we introduce these special rules for papers reporting crystal structures.

1. Crystal data on each structure containing organic carbon should be deposited with the Cambridge Crystallographic Data Centre (CCDC) to the following electronic address: deposit@ccdc.cam.ac.uk. Instructions can be found on the website www.ccdc.cam.ac.uk. Structural data are freely available from the Cambridge database upon request through the web page www.ccdc.cam.ac.uk/data_request/cif.

   The deposition number(s) and the web address should be mentioned in the manuscript. Typically, the following phrase will appear in the Experimental section: "CIF file containing complete information on the studied structure was deposited with CCDC, deposition number 626122, and is freely available upon request from the following web site: www.ccdc.cam.ac.uk/data_request/cif". When crystal structure data are listed in a Table in the manuscript, the deposition number(s) should be included in the Table (for each reported structure).

2. CIF files of the studied structures should be submitted to the Editorial Office together with the manuscript for the purposes of reviewing. The files may be created using the program enCIfer which is freely available from the web page http://www.ccdc.cam.ac.uk/products/encifer/index.html. Prior to the submission, each file should be checked for the absence of "warnings of types A, B and C" using the program checkCIF which is available from http://journals.iucr.org/services/cif/checking/checkfull.html. The referees can check the presented CIF file and suggest returning the whole manuscript back to the authors for revision if the program still generates warnings of type A. Warnings of types B and C require clarifying comments in the manuscript.

3. Tables of atomic coordinates of structures deposited with CCDC may be placed in the paper only if they are not longer than one page and necessary for discussion. Full Tables of interatomic distances and valent angles may be included in the paper only in exceptional cases and only if they do not exceed, in total, one page. Only most important for discussion bond lengths and angles are recommended to be included in form of a short Table, in the text or in Figure captions. Instead of a long list of same-type bonds and angles, only ranges showing the variation of the values, or the corresponding average values, should be given.

4. Complete crystal structure data should be reported for inorganic structures studied.

5. In the Experimental section, basic crystal structure parameters (structural/refined stoichiometry; molecular mass; crystal system; space group; unit cell parameters; the number of formula units per unit cell; calculated density) and essential parameters of the XRD experiment (experimental temperature; size, color and shape of the crystal(s); the number of total measured and unique utilized reflections; R-value(s) for equivalent reflections; the number of refined parameters; the final value(s) and type of R-factor; goodness of fit; residual extrema; absorption coefficient for structures with heavy atoms; absolute structure parameter for chiral crystals) should be listed in a Table or in the text. The Experimental section should also report on how the crystals were selected, type of instrument and radiation, theta-range, if and how absorption correction was applied, as well as any non-standard details of the experiment. Then the methods and programs used in the structure solution and refinement should be mentioned including the description on how positional and thermal parameters of hydrogen atoms were refined, if constraints/restraints were applied (for example, for disordered fragments), if the rigid-body model was applied and if any non-standard methods were used in the course of solution/refinement.

   The results of a powder XRD experiment should comprise crystal structure data (unit cell parameters, atom coordinates, site occupation factors, basic interatomic distances, quantitative ratio of available phases in the studied sample, etc.) and should be supported by independently obtained data on the chemical composition of the sample.

6. When a paper reports one crystal structure only, it will be presented as "Short communication" and should fit, with all Tables and Figures, in no more than three journal pages. When a paper reports additional data or more than one crystal structure, and assigned by the Editors to "Short Communications", it should fit in no more than four pages.