Journal of Structural Chemistry

Author Guidelines

1. General Info

The Journal of Structural Chemistry (JSC) reports new experimental and theoretical research and reviews in Russian and in English to present results in the following areas of structural chemistry: theory of molecular structure and chemical bonding; physical methods in molecular structure research; structure of liquids and solutions; crystal chemistry; supramolecular compounds and nanosystems; structure of biologically active systems; structural aspects of functional materials.

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The affiliations, full postal address, e-mail address, and, if possible, the unique ORCID identifiers should be indicated for all authors. The ORCID identifier must be specified for the corresponding author.

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The following materials are to be submitted to the Editorial Office to publish the article:

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The following information should be specified along with the manuscript: title of the article, names of authors, addresses of scientific institutions, short abstract, and key words *in English*.

Manuscripts are reviewed anonymously in terms of their relevance, scientific value, compliance with the scope of the Journal and with these Guidelines. Based on the reviewers' comments, the Editorial Board makes the decision about the possibility and the terms of publishing the article (without revision; revision is required; major revision is required within one month; article is declined). The article is to be revised according to the reviewers' comments and resubmitted together with corresponding responses to the reviewers.

The Editorial Board reserves the right to make minor reductions or changes to the text of the article without distorting its scientific integrity.

The galley proof of the article is sent to the corresponding author's e-mail. The corrections, if necessary, should be submitted to the editorial office within two working days.

After the article is published, its electronic copy (a PDF document) is sent to the authors.

2. Manuscript Format

The Journal accepts two types of manuscripts: an article (a full paper) or a review.

The manuscript should begin with the title followed by initials and surnames of authors, full affiliations, zip codes, addresses, and the e-mail of the corresponding author. Then specific results and conclusions should be provided in a short abstract (no more than 20 lines), followed by several (up to 10) keywords to describe the research area and the obtained results. Example of the first page of a manuscript (see Suppl. 1)

The manuscript ends with a list of references in the order of their appearance in the text.

If necessary, the authors can express their acknowledgements in a separate paragraph before the list of references.

The authors may submit supplementary materials, which will be posted electronically "as is" at the JSC website **http://jsc.niic.nsc.ru** and at the Springer website **https://link.springer.com/journal/10947**.

Review articles

The review should represent/describe the state of modern research in a particular field of structural chemistry and provide an objective critical analysis of the literature available on this subject.

Articles

The article should clearly describe the results of the research aimed at solving some relevant fundamental scientific problem; it must contain scientific novelty.

The authors are suggested to divide an article into the following subsections: Introduction, Experimental, Results and Discussion, Conclusions.

In the Introduction, it is appropriate to mention closely related works of other authors, including those published in domestic journals, and the works that appeared over the past two or three years, formulate the aim of the work and justify the relevance and the fundamental importance of the presented research. The Experimental part should describe the investigated compounds (materials), instruments, software, methods, and measurement techniques. When presenting and discussing the results, it is should be clearly distinguished between the results obtained in this work and those from earlier works (cite references).

The information presented in the figures or in the tables should not be duplicated.

3. Manuscript Preparation

This section presents general formatting requirements for submitted articles. The text of the article must be typed using standard Times and Symbol fonts.

References are cited in square brackets. For example: compound **2** was synthesized according to the published procedure [1].

When submitting the electronic version of the article, the authors attach the original Word (or RTF) document as well as the PDF document.

Units of measurement, chemical nomenclature, abbreviations

The authors should use the International System of Units (SI) and follow IUPAC recommendations. All abbreviations and acronyms (except for those commonly agreed) should be explained at their first appearance in the text. If the number of the abbreviations is high, they should be explained in a separate list after the keywords. A decimal point is used to separate fractional parts of decimal numbers (e.g., 3.14).

Tables

Each table must be numbered and have a title. A dash mark is used to indicate the lack of data. The number of significant figures in the tables should correspond to actual measurements or calculation errors. Tables can be accompanied by footnotes and comments.

Figures

Illustrative material is sent to the editor in separate files:

- Photos in bitmap formats (BMP, TIFF, PNG, JPG). The resolution must be no less than 300 dpi (preferably at least 600 dpi).
- Graphs, figures, chemical structures in the vector format (WMF, EMF, EPS, CDR versions up to 13) and in the format of the program in which they were made. The EPS format must be prepared with converting fonts to curves. Figure captions must be made in Times New Roman, size 9; line thickness no less than 0.18 mm (0.5 pt). For the design of chemical structures we recommend to use the ChemDraw program.

Colored figures are published only in the electronic version of the journal. The authors need to make sure that in black and white printing the illustrations do not contain additional background and remain informative: the lines are clear, digits and symbols are easy to read. It should be noted that tints can differ in the published colored figure from the original.

The figure width should not exceed 16 cm; the height should not exceed 23 cm. It is not recommended to give unnecessary details and inscriptions in the figures. It is recommended to replace inscriptions by digits or letters and interpret them in figure captions. It should be taken into account that figures and schemes can be diminished in layout setting, therefore they must not be overloaded with information and have parts that strongly differ in scale.

Figure captions are given in English. It is forbidden to use Russian words or designations.

When necessary, the editor can ask the authors to send a figure of a higher quality or in another format.

In the Word file of the article, figures and tables are given at the end of the text with their enumeration. If there are several parts of one illustration, they must be placed after each other. Each figure or table should be mentioned in the text, and their intended location is marked by a separate line. Chemical structures can be inserted directly into the text of the manuscript. Figure captions are presented on a separate page.

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Mathematical formulas

Simple mathematical formulas can be typed directly in the text of the manuscript or placed on separate lines with or without numbering. Cumbersome mathematical notations should be avoided. For example, it is recommended to use fractional exponents rather than a root sign, the "exp" symbol for exponential dependence, a slash for fractions, etc. Equations are placed on a separate line, and their numbers near the right margin. Formulas and equations should be numbered only if cited in the text. For example:

$$\Delta E = E(\mathrm{A;B}) + E(\mathrm{A+1;A}) - E(\mathrm{A+1;B}) \qquad (1)$$

References

References to the literature should be numbered by order of their appearance in the text and listed at the end of the article; text citations are presented as a sequence number within square brackets. References can cite scientific articles published in the journals referenced by known databases (WoS, Scopus, Russian Science Citation Index), monographs, books, software, known databases. All authors must be cited, using *et al*. instead of the names of authors is not allowed. Journal title abbreviations should correspond to those used by the *Chemical Abstracts Service Source Index*. If a Russian journal has a translated version, it is necessary to refer to the English version. It is desirable to specify DOI for all publications. To facilitate the search for DOI, you can use the Crossref service https://apps.crossref.org/SimpleTextQuery. References to articles and patents indicate their titles.

Authors are responsible for the accuracy and completeness of all references. The Editorial Office encourages the authors to double-check the list of references according to the original document.

Examples of references:

Article: S. Mochizuki, T. Kitao, T. Uemura. Controlled polymerizations using metal–organic frameworks. *Chem. Commun.*, **2018**, *54*, 11843. https://doi.org/10.1039/C8CC06415F

Article accepted for publication: A. Gal, R. Wirth, Z. Barkay, N. Eliaz, A. Scheffel, D. Faivre. Templated and self-limiting calcite formation directed by coccolith organic macromolecules. *Chem. Commun.*, accepted. https://doi.org/10.1039/C7CC03639F

Monograph: D.D. Perrin, W.L.F. Armarego, D.R. Perrin. Purification of Laboratory Chemicals. UK, Oxford: Pergamon Press, **1980**.

Edited books: Reviews in Computational Chemistry / Eds. K.B. Lipkowitz, D.B. Boyd. New York: VCH, **1996**.

Article from an Edited book: M.N. Sokolov, N.G. Naumov, P.P. Samoylov, V.P. Fedin. Clusters and Cluster Assemblies. In: Comprehensive Inorganic Chemistry II / Eds. K.P. Jan Reedijk, K. Poeppelmeier. Oxford: Elsevier, **2013**, Ch. 2.11. https://doi.org/10.1016/B978-0-08-097774-4.00212-6

Otherwise: M.N. Sokolov, N.G. Naumov, P.P. Samoylov, V.P. Fedin. Clusters and Cluster Assemblies. In: Comprehensive Inorganic Chemistry II / Eds. J. Reedijk, K. Poeppelmeier. Oxford: Elsevier, **2013**, Vol. 2, 271–310. https://doi.org/10.1016/B978-0-08-097774-4.00212-6

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A.N. Kravchenko. Biciklicheskie bismocheviny, ih predshestvenniki i analogi (Bicyclic Bisureas, Their Precursors and Analogues): Doctoral/Cand. (Chem.) Dissertation. Moscow: Zelinsky Institute of Organic Chemistry, **2007**. (In Russ.)

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The Sadtler Standard Spectra: 300 MHz Proton NMR Standards. Philadelphia, PA: Bio-Rad, Sadtler Division, **1994**, No. 7640 (1-Chloropentane).

Patent: S.K. Sheem. Low-Cost Fiber Optic Pressure Sensor. US Patent 6738537, **2004**.

Online edition: M. Zloh, D. Esposito, W.A. Gibbons. Helical Net Plots and Lipid Favourable Surface Mapping of Transmembrane Helices of Integral Membrane Proteins: Aids to Structure Determination of Integral Membrane Proteins. *Internet J. Chem*., **2003**, *6*, Article 2, http://www.ijc.com/articles/2003v6/2/ (accessed Oct 13, 2004).

Graphical Abstract

An informative color image no larger than 65*40 mm in size and no less than 300 dpi in resolution, which captures the essence of the article in graphical form, should be submitted by the authors for the illustrated content of the issue. Texts can be used in the graphical abstract only in case of extreme necessity (formulas, equations, etc.), any duplication of the article title or abstract should be avoided.

Structural formulas

Structural formulas should be created using special software such as ChemDraw, ISISDraw, or ChemWindows and can be inserted into the Word document as an image. If other software products are used, the structures must be first saved in one of the acceptable graphic formats and then inserted into the Word document.

Description of new compounds

The single-crystal X-ray diffraction data alone are not an unambiguous characterization of new compounds. The compounds should also be characterized by spectroscopic and analytical methods suitable for this particular sample or compound. Other methods can include elemental analysis to support the phase purity and composition, NMR spectroscopy, mass spectrometry, infrared and electron spectroscopy.

Description of crystal structures

The amount of data in tables should be minimized. The experiment can be briefly described using a table of crystallographic parameters and the information required to collect and refine the data.

Before submitting the manuscript, the authors should check the quality of their CIF files using the checkCIF website of the International Union of Crystallography (http://checkcif.iucr.org) and upload the checkCIF output (combined into a single PDF document) as a supporting information for the reviewers. Any warnings of A and/or B level must be addressed before submitting the manuscript and explained in the checkCIF PDF document.

Before submitting the manuscript, CIF and FCF files, the tables of structural factors, and CheckCIF reports must be sent either to the Cambridge Crystallographic Data Center (CCDC) or, in case of purely inorganic substances, to FIZ Karlsruhe (ICSD) (https://icsd.fiz-karlsruhe.de). The CCDC or ICSD number(s) are to be indicated in the manuscript.

Supplementary: article format for the papers reporting crystal and molecular structures

Due to a growing amount and standardization of structural data and the increasing role of electronic resources, the articles presenting X-ray diffraction analysis of single-crystals or polycrystals should be formatted according to the following rules.

CIF files of the studied structures should be submitted to the Editorial Office together with the manuscript so that the structural data could be reviewed. CIF files can be made using the *enCIFe*r editor available online at http://www.ccdc.cam.ac.uk/products/encifer/index.html. Any warnings of A and/or B level must be addressed before submitting the manuscript and explained in the checkCIF PDF document.

The Experimental part must be provided in a concise tabular or text form the main crystal structural data (composition, molecular mass, crystal system, space group, unit cell parameters, number of formula units in a cell, calculated density) and the main parameters of the X-ray experiment (temperature of the experiment, size, color and shape of the crystal, absorption coefficient, number of measured and unique reflections, *R*-factor for equivalent reflections, number of refined parameters, final value and the type of *R*-factor, quality factor of fitting and the magnitudes of the residual stress extrema on the electron density map, as well as the absolute structure parameter for optically active crystals). The Experimental part must also specify the conditions of

crystal sampling, the type of the diffractometer and the radiation, the range of data collection, completeness of obtained data, absorption corrections and any non-standard details of the experiment. Further, the Experimental part should specify which methods and program packages were used to solve and refine the structure, how positional and thermal parameters of hydrogen atoms were refined, whether additional conditions were imposed on the values of the refined parameters (e.g., for the fragments of disordered structures), whether the model of rigid body was used and any non-standard solutions applied to determine the structure. The results of polycrystal X-ray diffraction studies should present structural data (unit cell parameters, atomic coordinates, population of positions, main interatomic distances, quantitative phase relationships, size of coherent scattering regions, etc.) and should be accompanied by independent data on the chemical composition of the sample.

Supplement 1. Example of the first page of a manuscript

A DFT STUDY ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF SMALL TOXIC GASES ON B- AND Al-DOPED C_{20} FULLERENE

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Received *Revised*

The structural and electronic properties of semiconducting BC_{19} and AlC_{19} heterofullerenes as adsorbents for toxic small gas molecules (H_2S and SO_2) are determined by DFT. Structural parameters, energy gaps, natural population analysis, partial density of state, dipole moments, and vibrational frequencies were extracted. The adsorption process and sensitivity to the gases are increased by doping with B or Al. The results show that AlC_{19} is the most sensitive structure. The good sensing of AlC_{19} is related to high charge transfer upon gas adsorption. Adsorption of the H_2S on the BC_{19} has negligible effects on the electronic properties, to be categorized as "harmless adsorption". H_2S is weakly adsorbed on BC_{19} and AlC_{19}. The H_2S and SO_2 molecules act as electron donating and electron withdrawing molecules, respectively. Notably, the adsorption processes are highly exothermic. In general, BC_{19} is more reactive than C_{20} and AlC_{19} is the most reactive cage. This provides a theoretical basis to fabricate B- and Al-doped C_{20}-based gas sensors.

DOI: 10.15372/JSC20170403

K e y w o r d s: heterofullerene, electronic structure, toxic gas sensing, DFT.

In the Introduction, it is appropriate to mention closely related works of other authors, including those published in domestic journals, and the works that appeared over the past two or three years, formulate the aim of the work and justify the relevance and the fundamental importance of the presented research. The Experimental part should describe the investigated compounds (materials), instruments, software, methods, and measurement techniques. When presenting and discussing the results, it is should be clearly distinguished between the results obtained in this work and those from earlier works (cite references).