Instructions to Authors

South African Journal of Chemistry

Publication Policy: The South African Journal of Chemistry publishes original work in all branches of chemistry. Contributions, in English, may take the form of research articles, short communications or critical reviews. Prospective authors are invited to submit their manuscripts online at http://www.saci.co.za/journal/. Authors are strongly advised to observe the requirements of the Journal’s house style, as described below, paying particular attention to the Guidelines for Article Formats. Manuscripts not complying with these requirements will be returned to the authors for reformatting. Independent referees assess all manuscripts.

SAJChem applies the Creative Commons Attribution (CC BY) license to manuscripts we publish. This license was developed to facilitate open access – namely, free immediate access to, and unrestricted reuse of, original works of all types. Under this license, authors agree to make articles legally available for reuse, without permission or fees, for virtually any purpose. Anyone may copy, distribute or reuse these articles, as long as the author and original source are properly cited. Additionally, the journal platform (http://saci.co.za/journal/) that SAJChem uses to publish research articles is Open Access. We are registered with the Directory of Open Access Journals (DOAJ) and Scientific Library Online (Scielo).

It is a CAS-abstracted publication and is listed in Current Web Contents, Web of Knowledge, etc. It is an accredited publication with the South African Department of Higher Education and Training.

Authors bear sole responsibility for the factual accuracy of their publications. The use of electronic technology at all stages in the publication process leads to rapid publication times, and wide dissemination of the research presented. All papers are published online in PDF format.

Plagiarism policy: The journal scan each submission for plagiarism. Authors will be given the opportunity to rectify minor potential similarity issues. Suspect cases of more serious nature will be declined with reasons and authors are flagged. Authors can contact the Editor-in-chief to clarify any issues about potential plagiarism issues. If authors are flagged twice, without clearing these issues with the Editor-in-chief, their accounts with the journal will be disabled.

Language Editing services: Authors whose first language is other than English are particularly encouraged to seek the advice of a competent English speaker in reviewing their manuscripts before submission, with a view to improving grammar, spelling, usage, etc. The Journal does not provide language editing service. Links to several language editing services are provided. The South African Journal of Chemistry does not have any preferences for the use of any particular service provider.

• http://www.bioedit.co.uk
• http://www.biosciencewriters.com/
• http://www.charlesworthauthorservices.com/~BIOCHEMIA
• http://www.editage.com/
• http://www.enago.com (additional information)
• http://www.koonec.com/
• http://webshop.elsevier.com/languageediting/
• https://help.plagtracker.com
• http://www.prof-editing.com/index.php
• http://www.regentediting.com
• http://www.umna.hr/Savjetovanja_en.html
• http://www.writescience/right.com/
• http://www.360researchpapers.com
• http://www.24x7editing.com
• http://proofreading.org
A Research Article is a comprehensive contribution to the subject, and includes all essential experimental information and a critical discussion of results. Introductory material and background discussion should be terse and relevant. Although brevity is encouraged, a long but cohesive paper is more acceptable than fragmented accounts on a single theme. A Short Communication is a concise account (ca. 1500 words) of novel and significant results of which urgent publication is warranted. Short communications will be processed as expeditiously as possible. A Review is an authoritative and critical account of recent and current research in a specialized field, to which the author has made notable contributions. Prospective authors are requested to submit a suggested topic and a brief outline of the scope of the review to the Editor-in-Chief before writing it. On submitting material for publication, authors are encouraged to supply the names and e-mail addresses of two or three potential referees. The editors reserve the right to approach these nominated referees, or not, at their discretion. Authors submitting work for publication are required to complete and sign an exclusive copyright transfer form, without which publication may not proceed. Copyright transfer forms may be printed, completed, signed and either posted or faxed to the Editor-in-Chief at the address given below.

Papers describing new synthetic methods: Authors need to include a table in which representative examples of the reactions that were investigated are compared with the best synthetic reports in literature. The table heading should make it clear that it contains representative examples and that it contains data for comparison with the best methods in the literature. References, conditions, yields etc. should be included in the table. The paper must also include a table in which the scalability (up to 1g, higher if possible) of the reaction is demonstrated. This table should include representative examples (about a third) of the reactions that were investigated. Include a paragraph or more in which a motivation is provided on the merit of the new method in the light of the existing methods in literature (advantages versus disadvantages). The reader should be convinced why this is a better method than previous methods. If TLC was used, please provide the TLC conditions and Rf values. Authors should also provide proton and NMR spectra for all the compounds that are reported as supplementary material for review purposes. This should be uploaded as one PDF file with the submission of the paper.

Analytical Chemistry papers: This journal accepts investigative research papers which report studies concerning the development of analytical methodologies and/or novel applications. Scrutiny will be placed on the significance of the research and the extent to which it adds, or supports existing knowledge in the area when determining its suitability for publication.

Submissions detailing fundamental research on all aspects of analytical theory and methodology, such as innovative instrumental, chemical and biological approaches, detectors and sensors, sample treatment methods and data treatment are encouraged. Submissions telling the use of routine analytical methods or straightforward extension of these methods to new sample matrices will normally not be published unless a degree of novelty is highlighted. This has to be demonstrated to give very clear and quantifiable advantages over previous reported methods. Papers that report use of new sorbents are welcome provided that they show quality assurance information as given below. Authors should address the question of how their proposed methodology compares with previously reported methods and the method should comprise information on selectivity and/or quality assurance parameters (recovery, sensitivity, detection limits, accuracy, and reliability). Proper statistical treatment of the data should be provided.

Analytical/Physical chemistry papers – additional requirements: Please ensure that you indicate for each applicable graph/figure and table the number of times that the experiment was repeated to obtain the reported values. Also incorporate standard deviation/%error where required. Ensure that this information (number of times repeated) is also included in the respective experimental sections.

Nano- and materials chemistry papers: Ensure that sufficient characterisation of the materials under investigation is presented.
Novel compounds: If new compounds are reported, the paper should include suitable discussion of the IR, NMR and MS spectra to convince the reviewers/readers that you have correctly elucidated the structure of the compound(s). The paper must also preferentially include elemental analysis confirmation of the purity of the sample, or if not possible (in case of oily samples), HRMS data. The authors should also upload the IR, NMR (at least proton and carbon spectra) and MS spectra as supplementary material.

Characterization of novel materials and products: All novel products should be characterized with standard methods. Catalytic, adsorbent, and nano-materials used should also be thoroughly characterized with standard methods from the specific field of study.

Papers containing Bioassays: For bioassay data, be sure to include a reference drug so that the reader can compare the activity of the compounds tested. Also include a section (with references) on the statistical analysis that was used to treat the data. Include the number of times the experiment was repeated and what the %error for each reading was (in the experimental section and where the results are presented). Authors are also required to provide cytotoxicity results for the compounds that show promising bio-activities.

Lay-out of Manuscripts: Manuscripts should be prepared using one of the standard word-processing packages, e.g. Microsoft Word, Word Perfect or Open Office. All papers should have the following general structure:

a. Title, which should be concise but sufficiently informative for information retrieval purposes.

b. Authors’ names (one given name, initials and surname of all authors) followed by their full address(es). Use a normal footnote to indicate the details of the corresponding author (*To whom correspondence should be addressed. E-mail: email address)

c. Abstract of no more than 200 words in English. The abstract should not contain information which is meaningless without referring to the text; thus equation and formula numbers should be avoided unless qualified by an adequate description. Do not refer to illustrations, tables and literature. For short communications the abstract should be limited to one or two short sentences.

d. The Abstract should be followed by up to five Keywords.

e. The paper may be organized under main headings such as Introduction, Experimental, Results and Discussion, (or Results, Discussion), Conclusions, Acknowledgements and References. Experimental and Results and Discussion should have appropriate subsections. All tables and Figures should be part of the text and put at appropriate place.

f. In short communications the text should not be interrupted by headings, but essential experimental information should be given under the heading Experimental. Note that the References section should be prepared strictly in accordance with the Instructions, as the electronic conversion process uses EXACTLY what is provided by the authors in the submission (see the format for References below).

g. Manuscript pages should be numbered consecutively.

Content of Manuscripts: Authors should follow IUPAC rules for nomenclature and the International System of Units (SI) as far as possible. Familiar abbreviations may be used, but should be defined once if any doubt exists. Experimental data for organic and inorganic compounds should be presented in a consistent manner; the preferred sequence for reporting the new data is: m.p., [α]D, λmax, ε, νmax, m/z (Found: C, H, N, %. Calc. for CwHxN,yO,z: C, H, N, %). Authors should ensure that exact masses quoted for the identification of compounds should be accurate to within 5 ppm (EI and CI) or 10 ppm (FAB or LSIMS) and that for elemental analysis an accuracy of 0.3% is required. Superfluous data, e.g. m/z and νmax details, which are not structurally significant, should be omitted. Novel preparations of known compounds should be accompanied by a literature reference and significant comparative data, e.g. lit.³ m.p., [α]D. Standard preparations of known compounds are unnecessary, and repetitive descriptions of similar procedures should be avoided. In the latter cases one typical description will suffice, and may be accompanied by tables of analytical and spectral data.
**Experimental section:** It should be clear from the experimental section which of the compounds/materials are novel. Authors should explicitly mention if this is the case. If compounds/materials are not new, then authors should indicate if the data reported corresponds to previously reported data, providing citations for the original results. In general, please provide literature support for the methods that were used.

Authors should provide the model number and supplier of equipment that was used. Ensure that the experimental details for all results are provided. As far as possible, refer to tables and figures where the results are presented.

Ensure that generally accepted methods of analysis (as far as possible state-of-the-art methods of analysis) are provided for all new compounds/materials. IR, NMR, MS and elemental analysis data should be provided for new compounds. High resolution mass spectrometry data can be used for the latter (for example when the compound is an oil). Authors should indicate how the product was purified (chromatography, recrystallization, HPLC etc.) Also provide the TLC conditions and Rf values if applicable. If the compound is a solid, the melting point should be provided.

If the compounds reported are not new, spectral data, melting points are only required for key entities – cite literature where the data was published and compare melting points with reported literature values. For other known compounds, reference to the literature for method of synthesis and the spectral data is required.

**Example of the listing of spectroscopic data**

From the reaction of 4a with methyl iodide N-methyl-2-phenyl-1,4-benzoxazepin-5(4H)-one 5a (80%) was obtained as a semi-solid (m.p 85 °C); δH (400 MHz, CDCl3): 3.33 (3H, s, CH3), 6.29 (1H, s, 3-H), 7.13 (1H, d, J 8.1 Hz, 9-H), 7.20 (1H, t, J 7.6 Hz, 7-H), 7.31 (1H, t, J 7.3 Hz, 4'-H), 7.37 (2H, d, J 7.8 Hz, 2'-H and 6'-H), 7.42 (1H, dt, J 1.7 and 7.8 Hz, 8-H), 7.64 (2H, d, J 8.1 Hz, 3'-H and 5'-H) and 7.91 ppm (1H, dd, J 1.6 and 7.6 Hz, 6-H); δC (100 MHz, CDCl3): 36.5 (CH3), 116.5 (C-3), 120.2 (C-9), 124.1 (C-2' and C-6'), 124.9 (C-7), 126.9 (C-5a), 128.4 (C-4'), 128.6 (C-3' and C-5'), 132.1 (C-6), 133.1 (C-1'), 133.4 (C-8), 147.6 (C-9a), 160.5 (C-2') and 166.7 ppm (C-5); νmax (CHCl3): 1640 cm⁻¹ (CO); m/z: 251 (M+, 59.5), 210 (100), 181 (43.9), 105 (84.6), 77 (81.2) and 42 (86.9) (Found: C, 76.50; H, 5.52; N, 5.50%. Calc. for C16H13NO2 (251.28): C, 76.48; H, 5.21; N 5.57%).

**Computational or theoretical papers or any paper containing computational work in part.** The same format should be used, but a section "Theoretical Approach/Methods/Computational Details" should be added to the normal "Experimental" section, were applicable. In this section authors must provide a concise description of the computations in paragraph form, referring to the full level of theory/treatment and computational program or programs used. In addition, authors should ensure that Supplementary Material is provided (see Supplementary Material section below). This supplementary information will appear at the end of the manuscript, and will be available online. For standard quantum mechanical (i.e. DFT, ab initio or semi-empirical) calculations sufficient information must be included here to enable readers to reproduce the computed values. This must include the Cartesian or internal coordinates of final structures, accessible as ASCII data. Authors are also encouraged to include an example of an input file or input files, especially when non-standard features (e.g. user-specified DFT functionals, externally provided basis sets, non-default convergence criteria or DFT integration grids, advanced convergence routines) were used. The aim is not only to provide information for others to reproduce the values precisely, but also to enable readers to extract detailed structural information as required. Tables and/or figures should be clearly arranged, each with sufficient captioning to explain the information. If there is a strong reason for including previously published values in this information, the original sources should be properly cited in footnotes to
Tabs. Tabulated values should be accessible as ASCII data or readily translated to ASCII so as to allow readers to extract data for other computational purposes.

**Tables** should be numbered consecutively in arabic numerals (e.g. Table 1) and should bear a short, yet adequate caption. Also ensure that each table is self-explanatory. Footnotes to tables should be designated by lower-case letters which appear as superscripts to appropriate entries. Tables should be in a readable form not exceeding one page. Column headings should be organized such that they represent a physical quantity divided by its unit, e.g. T/K, so that the entries in the columns are dimensionless. Columns of integral numbers should be right-justified, and floating-point numbers should be aligned according to their decimal points. Tables should be prepared using the Microsoft Word table function, rather than using tabulations. **Tables should be positioned in the text at the most suitable positions.**

**Example of the format of tables**

**Table 3.** Influence of interferences at 25 °C.

<table>
<thead>
<tr>
<th>Metal ion</th>
<th>Concentration of interferent/mg dm$^{-3}$</th>
<th>Zinc found/mg dm$^{-3}$</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe$^{3+}$</td>
<td>50</td>
<td>51.8</td>
<td>3.8</td>
</tr>
<tr>
<td>Cu$^{2+}$</td>
<td>50</td>
<td>50.4</td>
<td>0.8</td>
</tr>
<tr>
<td>Ni$^{2+}$</td>
<td>50</td>
<td>52.3</td>
<td>4.6</td>
</tr>
<tr>
<td>Pb$^{2+}$</td>
<td>50</td>
<td>51.2</td>
<td>2.4</td>
</tr>
<tr>
<td>Co$^{2+}$</td>
<td>50</td>
<td>51.2</td>
<td>2.4</td>
</tr>
</tbody>
</table>

**Equations** should be numbered consecutively using parentheses arabic numerals flush with the right-hand margin. When numbering, make no distinction between chemical and mathematical equations. Equations should commence at the left-hand margin, signs should be spaced, and no more than 50 characters (including spaces) should occupy each line in the manuscript. All equations must be generated using specialised software (e.g. ChemDraw or Microsoft Equation). Equations should be placed in the text at the most suitable positions.

**References:** An Endnote template file is available if you prefer to use the Endnote software for your paper. [Click here to download the Endnote template](#), then save it under the “Styles” directory of your Endnote software. Please contact the Editor-in-Chief as given on journal website if you experience any issue. References should be numbered consecutively in order of appearance in the text, as unparenthesised superscripts to the right of any punctuation, and should be listed at the end of the paper. Journal references are given by initials and surnames of all authors, *journal title*, year, volume, first page - last page; book references by initials and surnames of all authors, *title* (initials and surnames of all editors followed by ed. or eds.), volume, edition, publisher, city or cities, country, date, page(s); thesis references by initials and surnames of the author, *title*, kind of thesis (e.g. “PhD thesis”), university, city, country, publication year; software references by initials and surnames of all authors, program name and version, publication year, institution, city, country. Titles of journals should be abbreviated according to Chemical Abstracts practice (see [http://www.cas.org](http://www.cas.org)). Authors should avoid using footnotes. Some typical examples are presented below:

(Note that from 1 January 2015, references to journal articles should include the title of the manuscript.


7. G.M. Sheldrick, SHELXTL Ver. 5.03, 1996, Institut für Anorganische Chemie, University of Göttingen, Göttingen, Germany.

**Figures and Illustrations** should appear in the text at the most appropriate positions. Also ensure that each figure/graph is self-explanatory. There are no restrictions on the use of colour for articles appearing in the *South African Journal of Chemistry*; indeed authors are encouraged to make full use of colour graphics in order to enhance the presentation of their work. Graphics files should be prepared at a maximum width and height of 500 pixels, with white space being kept to a minimum, while retaining an opaque background, ensuring that lines have a uniform thickness and that lettering is of a size which will be clearly legible after reduction. Authors should use standard graphics computer packages; 300 dpi TIFF or high resolution JPG, ChemDraw and ChemWindows files, or preferably files in vector format, such as WMR, EMP or EPS, are preferred. Labels of the axes of graphs, like Table column headings, should represent a physical quantity divided by its unit, e.g. ln(k/dm$^3$ mol$^{-1}$ s$^{-1}$), so that the quantities on the axes are dimensionless. Figures should be numbered consecutively using arabic numerals (e.g. Figure 1), and descriptive captions should be included in the text immediately below the Figures.

**Structural formulae** should be drawn with the aid of standard computer packages, such as ChemWindows or ChemDraw, and individually designated by unparenthesized boldface arabic numerals corresponding to those in the text; roman numerals are not acceptable. Authors who use ChemDraw must use the built in ACS style when preparing structural formulae. Authors who use other drawing packages must adjust the settings so that they are as close as possible to the following specifications: bond length: 0.508 cm (14.4 point); double bond spacing: 18% of bond length; bond width: 0.071 cm (2 point); line width: 0.021 cm (0.6 point); hash spacing: 0.088 cm (2.5 point); chain angle: 120 °; font: Times New Roman 10 point. When several structural formulae are depicted, they should be grouped in logical blocks and not scattered throughout the text. Numbering should be consecutive if possible, and formulae should not be repeated if used in a later lay-out; the number will suffice. Blocks of numbered structural formulae do not usually require further designation. They should appear in the text at the most appropriate positions. Reaction and mechanistic sequences may be numbered and referred to as **schemes** if this facilitates discussion in the text. A descriptive caption is preferred when the scheme is numbered. For submission of structural formulae and schemes the same instructions apply as for the submission of Figures and Illustrations.

**Three-dimensional images** of, for example, results from molecular modelling or molecular orbital calculations may be displayed as 3D images, which allow readers to rotate, zoom in, etc. to inspect the figures more closely. These figures may be viewed using the Chime plugin (http://www.mdl.com/chemscape/chime/), or Cosmoplayer (http://ca.com/cosmo/). Acceptable file types include MDLI Mollfiles, xyz format, Brookhaven Protein Databank (PDB), Adobe 3D (U3D), MOPACInput, GaussianInput and VRML.

**Spectra**: Many software packages allow spectra, chromatograms, etc. to be saved in JCAMP-DX format. The file specifications for some of these packages are available free from the IUPAC Working Party on Spectroscopic Data Standards (JCAMP-DX) website (http://www.acornnmr.com/JCAMP.htm). Plots in JCAMP-DX format may then be displayed using the Chime plugin (see above), and expanded and manipulated on screen. This will be an additional feature located next to the spectra embedded in the paper. Providing JCAMP-DX files allows readers to save published spectra for direct comparison with their own spectra. Alternatively, copies of spectra may be supplied in PDF format as Supplementary Material.

**Crystallographic data**: Papers containing crystallographic data are assessed in terms of their chemical significance. However, sufficient data should be included to enable other workers to
reproduce and extend the calculations. The presentation of crystal data should conform to the recommendations of the Commission on Crystallography of the IUCr (Acta Crystallogr., 1967, 22, 445). Authors should submit for refereeing purposes and subsequent deposition (see Supplementary Material) all supplementary crystallographic data as a Crystallographic Information File (CIF), which should include anisotropic vibrational parameters and structure factor tables: these tables should not be numbered. Significant derived data, such as bond lengths, bond angles and torsion angles, with their estimated standard deviations, which are necessary for the discussion, should be tabulated for publication. Full details of the refinement should be included. Authors presenting molecular coordinates from crystallographic or modelling studies in their submitted articles should use PDB, MOLfile or xyz formats. While coordinates provided by most crystallographers normally come in SHELX format, conversion of SHELX to PDB format may be easily accomplished using SHELX93, Chem3D or Babel.

When reporting powder diffraction data a sufficient instrument description must be included. This enables other researchers to reproduce and/or improve upon the experimental data. The instrument description must include (as listed in the experimental section) the make and model of the diffractometer (for example, Bruker D8 Advance, PANalytical X'Pert Pro diffractometer), the radiation source and wavelength(s) (for example Cu Ka1, 1.540562 Å), the instrument power settings (kV, mA), incident and diffracted beam slits, filters and monochromators, the temperature at which data were collected, the 2θ scan range, measurement step size, and description of the detector. For data reduction authors are required to list the least-squares refinement program used and the source of the initial unit cell dimensions (for example determined experimentally, obtained from a crystallographic database or indexing program).

**Supplementary Material:** In certain cases, detailed compilations of data or calculations may be considered by the authors, or by the editors and referees, to be of limited interest to most readers. Authors may submit or be advised to submit such information as Supplementary Material, as was pointed out above for example spectra for new compounds and required cartesian coordinates for computational chemical papers. At the time of publication this will be made available for viewing and downloading on the website of the journal. For an example of the required format for supplementary material, see: https://journals.co.za/deliver/fulltext/chem/67/1/chem_v67_a31supp.pdf This version has examples of spectra, X-ray and computational data.

**Archiving and Compressing Files:** For ease of handling, text and graphic files may be archived and compressed into one single file. Authors are advised to use a utility such as WinZip for this purpose.

**Manuscripts for publication should be submitted** in electronic form. The text font used for the manuscript is not important since the text are completely changed in the process to make the proofs. All files to be submitted in machine readable form must be thoroughly checked for viruses before submission.

Receipt of an article will be acknowledged by the Editor-in-Chief by e-mail, and the article will be logged with a reference number, which authors are asked to quote on all subsequent correspondence regarding their papers. If no such acknowledgement has been received within a reasonable period of time, authors should confirm with the Editor-in-Chief whether their manuscripts have been received safely or not.

Acceptance of an article is confirmed by the appropriate Scientific Editor once the article has successfully passed through the refereeing process. Authors will be advised whether their manuscripts have been accepted, with or without revision, or rejected. Manuscripts requiring revision should be returned to the Scientific Editor within three weeks, failing which the manuscript will be considered to have been withdrawn. Such manuscripts, if submitted at a later date, will be regarded as new submissions, and will have to undergo the refereeing process once again. The editors reserve the right to make further changes to bring manuscripts up to the expected standards and to ensure conformity with the house style.
Proofs: The author will receive the proofs of an article for checking from the Technical Editor by e-mail. Authors are requested to return any proof changes to the Technical Editor within 48 hours. Articles published in the *South African Journal of Chemistry* may not be published elsewhere without the written permission of the South African Chemical Institute.

**Guidelines for Article Formats**

1. **General**

   The text font used for the manuscript is not important since the text are completely changed in the process to make the proofs.

2. **Research Articles**

   **Publication type is RESEARCH ARTICLE.**

   **Abstract**

   Headings and sub-headings should be numbered in the following manner, not exceeding three levels (for example):

   1. **Introduction**
   2. Experimental
      2.1 Chemicals
      2.2 Instruments
      2.3 title
   3. Results and Discussion
      3.1 title
      3.2 title
   4. Conclusion
      Acknowledgements
      References

   If the sections are short, their subheadings should be italic (not bold) and should not be numbered.

   Please note: Abstract, Abbreviations, Acknowledgements and References are not numbered.

   To view an example of the format of a Research Article, click on the full text of article no. 21, by Mingsong Hu and Paul P. Coetzee, volume 60 (2007), pp. 113-117.

3. **Short Communications**

   **Publication type is SHORT COMMUNICATION.**

   **Abstract** – maximum one or two short sentences (maximum of 30 words). Headings – for Experimental only, without numbering.

   To view an example of the format of a Short Communication, click on the full text of article no. 11, by Frank van der Kooy and J. J. Marion Meyer, volume 59 (2006), pp. 60-61.

4. **Reviews**
Publication type is **REVIEW**.

Formatting applies as described above (point 1) and numbering scheme as explained for Research Articles (point 2). **Reviews should have a table of content that corresponds to the chapters and subsections if any.** Draft review especially with title and table of content should be submitted to the chief editor to seek guidance whether it can be accepted for possible review process.

Please note: A Table of Contents (no numbering for this heading) should be given after the **Abstract**. **Abbreviations** should be included before **Acknowledgements**.


SAJC editorial team, 2018 (modified)