

# JOURNAL OF THE BRAZILIAN CHEMICAL SOCIETY

Revista da Sociedade Brasileira de Química

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#### 1. Introduction

The *Journal of the Brazilian Chemical Society (JBCS)* embraces all aspects of chemistry except education, philosophy and history. It is a medium for reporting selected original and significant contributions to new chemical knowledge. The Journal publishes Articles, Communications, Short Reports, Reviews, Accounts and Letters.

The reproduction of figures, schemes and photos already published in other publications, even if these materials have been published by the same authors, requires the copyright permission given by the editor house allowing the publication of the article in the *JBCS*.

For materials (figures, schemes, etc.) under CC-BY license, the copyright permission is not necessary, and the author must include in the manuscript the credits (attribution), see the example:

Figure 1. A binary phase diagram for eutectic mixture formation (figure from reference 12 with CC-BY attribution).

# 1.1 Manuscript types

Article should be comprehensive and critical accounts of a work in a given area. Although short articles are acceptable, the Editors strongly discourage fragmentation of a substantial body of work into a number of short publications.

Communication should be restricted to reports of unusual urgency and significance or interest. They should be submitted with a statement from the authors as to why the manuscript meets these criteria. A manuscript will not be accepted if, in the opinion of the Editors, the principal content has previously been released or published in any other medium. The communication should not exceed 1500 words or occupy more than 3 pages of the Journal. To estimate the length of a communication, an average sized figure is counted as 100 words and separate formulae and lines of a table are counted as 8 words per line, including headings and horizontal rulings. Title, authors' names and literature references are not counted.

**Short Report** is meant to be a concise terminal report of studies of limited scope. Manuscripts submitted as articles or communications may, in some cases, be accepted as short reports. The standard of quality expected in short reports is the same as in articles.

**Review** is normally invited by the Editors. However, the Editors welcome suggestions for reviews considered suitable for the Journal. Be aware that the **topics** (items) in the **Reviews** must be **numbered** with Arabic numerals. In order to help the Editors in the evaluation of the suitability of a proposed Review, the authors should previously submit by e-mail (help\_office@jbcs.sbq.org.br) the following items:

- A synopsis including a brief outline of the Review content;
- A statement explaining the relevance of the topic to be reviewed;
- A list of reviews recently published on the same or related areas, if any;
- A summary of the lead, corresponding author's academic career, highlighting her/his experience in the field:
- If the text is already prepared (with the above items have been considered by the Editors), an invitation for submission will be sent for the author;

A short Curriculum Vitae (max. 100 words) with photo for each author needs to be added in the end of the main document.

Acceptance of the synopsis does not guarantee publication of the final manuscript.

It is quite common, in Reviews, the reproduction of figures, schemes and photos already published in other works. Even

if these materials have been published by the same authors, copyright permissions need to be given by the editorial office.

**Account** are personalized reviews by individuals or their research groups, dealing with their (important) recent work, and is published only by invitation from the Editorial Board. Like the Review, it may include figures, schemes, structures, etc. The **topics** in the **Account** must be **numbered** with Arabic numerals.

In order to help the Editors in the evaluation of the suitability of a proposed Account, authors should previously submit by e-mail (help\_office@jbcs.sbq.org.br) a synopsis considering the following items:

- submission of a focused and readable text, covering current areas of interest for the Chemistry community;
- it is necessary to present topics or summaries of research in an emerging area of Chemistry, covering only the most interesting/significant developments;
- in the conclusion section, the discussion is about possible future approaches of the Account subject;
- a short Curriculum Vitae (max. 100 words) with photo for each author needs to be added in the end of the main document.

In case any reproduction of figures, schemes and photos already published in other journals is included, a copyright permission given by the editorial office of the publisher must be sent to *JBCS* office.

**Letter** is a medium for the expression of scientific opinions and views normally concerning material published in the Journal, but not for revision/update of the authors' own work. When a **Letter** polemical in nature is accepted, a reply from the implicated parties will be requested for publication alongside the original **Letter**. Contributions in this format are intended to be published as soon as possible. No Abstract is required for letters. They should not exceed one printed page in length.

# 1.2 Before Beginning the Submission

See JBCS Ethical Guides and Publication Copyright in our webpage: http://jbcs.sbq.org.br/ethical\_guides

#### **1.3 ORCID**

The authenticated ORCID iD is required for the submitting agent. For those that do not have an ORCID identifier, the ScholarOne submission system is integrated to the ORCID website, and an account can be easily created during the submission process.

# 1.4 Collecting Author Contribution in the Submission

The ScholarOne-JBCS submission system is configured to use the <u>CASRAI's CRediT taxonomy</u> to recognize the individual contributions of authors (<u>containing 14 roles</u>), being a required item to the accomplishment of the submission. When adding authors to the submission, you will choose from a list of contributions. Check the author's role options, then select the level of contribution from the dropdown.

The <u>14 roles</u> according to the <u>CASRAI's CRediT taxonomy</u> are: Conceptualization, Data curation, Formal analysis funding acquisition, Investigation, Project administration, Resources, Software, Validation, Visualization, Writing original draft and Writing-review & editing.

The levels of contribution: Lead, Support, Equal.

#### 1.5 Collecting Author Contribution in the manuscript

For manuscript with <u>6 or more authors</u>, the JBCS requires the specification of the individual contribution of each author <u>in the text</u>. This information, according to the <u>14 roles</u> from the <u>CASRAI's CRediT taxonomy</u>, may be added before the Reference, named as Author Contributions, see <u>template</u>.

# 1.6 Anti-plagiarism Tool

The JBCS adopts the use of the anti-plagiarism Tool iThenticate since the end of 2015.

#### 1.7 Manuscript Organization

Authors should present their materials with the utmost conciseness and clarity. The **Introduction** should clearly and briefly identify, with relevant references, both the nature of the problem under investigation and its background. Extensive reviews of the literature cannot be accepted.

In **Articles** and **Short Reports**, the **Experimental** section may precede or follow the **Results and Discussion** section, but should be separated from it. The addition of a final section at the end of the manuscript, which briefly summarizes the main **Conclusions** of the work, is recommended and needs to be just after the **Results and Discussion** section.

**Descriptions of experiments** should be given in sufficient details to enable other researchers to repeat them. The degree of purity of materials should be given, as well as all quantities used. Descriptions of established procedures are unnecessary. Standard techniques and methods used throughout the work should be stated at the beginning of the section in a **Materials and/or Methods** subsection, in the **Experimental** section. Apparatus should be described only if it is non-standard. Commercially available instruments should be referred to by their suppliers and models.

All **new compounds** should be fully characterized, which includes spectroscopic data and elemental analyses. High-resolution mass spectra may substitute for elemental analyses if accompanied by unequivocal proof of sample purity (melting points, copies of NMR spectra, etc.). For compounds prepared in enantiomerically pure or enantiomerically enriched form, specific optical rotation must be given. In cases where enantiomeric excess is determined by chromatographic and/or spectroscopic techniques, copies of the appropriate chromatograms and/or spectra should be included as Supplementary Information upon submission of the manuscript. Data associated with specific compounds should be listed after the name of the compound concerned, followed by the description of the preparation, or else presented in tabular form in the **Results and Discussion** section. All spectra must be included in the **Supplementary Information** (SI, see Section 8).

Many theoretical and computational papers use a routine procedure based on a well-documented method, being it semiempirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers, in which the method has been developed, to cite the computer program used and to indicate briefly any modification made by the author. Complementary data meant to support the analysis of **Communications** should be included as **Supplementary Information** (SI, see Section 8).

It is the **authors' responsibility** to obtain permission from other publishers for the reproduction of artwork from other journals in the reviews or in any other type of publication. Such specific **Copyright Permissions** should be sent to the *JBCS* Editorial Manager. Suitable acknowledgement of reproduction must be given in the captions.

# 1.8 JBCS Polity Statements for Preprints

- The *JBCS* considers the submission of manuscript deposited in preprint servers.
- The Journal considers work submission both previously and simultaneous posted on a preprint platform.
- The *JBCS* does not authorize the posting of versions revised during peer review on a preprint server.
- The use of a preprint repository must be informed in the cover letter and in the submission platform, with the inclusion of the preprint link and DOI of the posted work.
- The preprint DOI (and link) needs to be cited in the reference list of the submitted manuscript.
- In case of acceptance of the paper in the *JBCS*, the preprint must updated with link of the publication.
- The authors are responsible for checking the compatibility between the license type chosen in the
  preprint server posting and the copyright of the article (this is assigned to the Sociedade Brasileira de
  Química (SBQ)).
- The *JBCS* draws attention to the authorship, for some license types of the preprint, the authorship must be the same in the repository and in the published in the Journal.

# 2. Preparation of Manuscripts

#### **General Overview:**

Font: Times New Roman

Font Size: 12
Font Color: Black

Spacing: double spaced

Pages: numbered consecutively

Tables, Schemes, Figures and captions: placed in the text, as close as possible to the first citation.

**Figures:** numbered with Arabic numerals. For full manuscripts containing material previously published in preliminary form, a copy of the previous communication is required and should be included at the end of the manuscript.

**Maps:** insert as **Supplementary Information** Main sections (Introduction, Experimental, Results and Discussion, Conclusion section) of the manuscript should NOT be numbered, EXCEPT for Account and Review.

**Supplementary Information (SI):** needs to be included at the end of manuscript, after the **Conclusions** section. It should contain RELEVANT and COMPLEMENTARY DATA to those presented in the manuscript. If new compounds are identified or characterized, **all spectra** should be included (see Section 8).

<u>Graphics/Figures/Schemes</u>: files should be uploaded in the system <u>individually</u>. *JBCS* preference is for files from original programs since editable files facilitate the correction of details out of JBCS standard. Some suggested extensions:

Structures in: \*.cdx (ChemDraw); Graphics in: \*.opj/org (Origin); \*.xls/xlsx (Excel); Others in: \*.cdr (CorelDraw); \*.tif/jpg (Paint), etc.

If you have worked with different programs, please write to <a href="help-office@jbcs.sbq.org.br">help-office@jbcs.sbq.org.br</a> informing which ones were used, and depending we may accept the files.

<u>Main document</u> (full): also keep tables/figures/schemes/equations and their legends <u>as close as possible of their first citation</u>.

Main document in: \*.doc/docx (Word); \*.tex (LaTeX, TeX).

# **Details:**

First Page

- Graphical Abstract (GA) (see Section 5)

Second Page

- Title
- Authors' names: full given name, followed by the middle name initial(s) and then by the full last name.

**An asterisk** (\*) should follow the name of the corresponding author.

- **Addresses:** Authors are asked to provide full addresses for correspondence. The e-mail address of the corresponding author should be given as a footnote. If the address where the work was carried out is different from the present address of any of the authors, a footnote indicating the current position can be included. Each address should have a correspondent letter. As for instance:

Jailson B. de Andrade,\* ,a Marta V. Andrade b and Heloisa L. C. Pinheiro c

# Third Page

**Abstracts:** maximum of 150 words for Articles, Accounts and Reviews and 50 words for Short Reports and Communications

**Keywords:** a minimum of three and maximum of five. Broad-sense words such as "water" should be avoided. The text should start from the third page of the manuscript.

Attention: all nomenclature should be consistent, clear, unambiguous and in accordance with the nomenclature rules established by the IUPAC, the International Union of Biochemistry, the Abstracts Service (see Index Guide to Chemical Abstracts, and <a href="https://iupac.org/what-we-do/books/color-books/">https://iupac.org/what-we-do/books/color-books/</a>), the Nomenclature Committee of the American Chemical Society or any other appropriate bodies. Units and symbols should follow IUPAC recommendations. Authors will not be denied any reasonable usage, but if non-SI units are used for critical data or for quantities measured to a high degree of accuracy, final numerical values should also be expressed in SI units.

Be sure that all abbreviations are once specified (as near as possible of their first citation).

# 3. Language, Style and Format

# Language

Only manuscripts written in **English** will be considered. Standard English and American English spellings are allowed but consistency should be maintained within the manuscript.

From now on, all authors are expected to send along with their manuscript a statement from a specialized company (or person), attesting that the text was submitted to **formal English review**. Otherwise, the Editor can, at any time, ask for such procedure to warrant the English precision, conciseness and understanding of the manuscript.

- Style and Format
- Main Sections: First initial with capital letter, bold, no final full stop. Should not be numbered, except for Reviews and Accounts:
- - Introduction

- - Experimental (or Methodology in case of theoretical and computational papers)
- Results and Discussion or Results then Discussion (alternatively, Experimental may follow Results and Discussion)
  - Conclusions
  - **Supplementary Information** (if you have): include the following text <u>just to mention</u> (<u>not to add graphs and data here</u>) the existence of the supplementary data, see the example:

# **Supplementary Information**

Supplementary data are available free of charge at http://jbcs.sbq.org.br as PDF file.

- Acknowledgments
- References
  - Sub-Sections: first initial with capital letter, no final full stop . Examples:

Reagents and equipments

X-ray data

- **Formulae (compounds):** should be numbered with bold Arabic numerals.
- **Structural** or **displayed formulae** must be accurately drawn and inserted in the text. All captions should be typed below the structural or displayed formulae, together with it, in the right position.

# 4. Guidelines for Illustrations

# **General Size**

The authors should think about the illustration size for double column (172 mm) of the journal. But, the font type size of text must be consistent with the illustration since it can be reduced during preparation of the Galley Proof.

This is important when choosing symbols for graphics, drawings, charts, photos, etc., be consistent, make your manuscript look nicer: use the same size and same font type in graphics, schemes, etc.

# 4.1 Graphs and Figures (also see Section 2)

**Lines and Lettering:** Lines should be black and of an adequate and even thickness. Solid, broke, dotted and dot-dash lines should be used in graphics. Particular care should be taken to ensure that the lines in a spectrum are of adequate thickness.

Lettering should not be smaller than 7 pt (Times New Roman) and lines not thinner than 0.5 pt. Lettering and lines should be of uniform density throughout the figures.

 $\textbf{Labeled atoms in ORTEP} \ (or \ any \ other) \ diagrams \ should \ have \ atom \ numbers \ in \ parenthesis, e.g., \ Fe(1), \ C(44).$ 

**Symbols** representing physical quantities should be given in italics, e.g., J (Hz),  $\delta$  (ppm), m/z, etc.

**Units** should be expressed in the appropriate form, e.g., g cm<sup>-3</sup> or mol L<sup>-1</sup>, rather than g/cm<sup>3</sup> or mol/L (see Section 4.5)

# **Graphs**

- Scales: graphs should have only the minimum necessary scale divisions marked by numerals.

- Axis labels should use SI units, separated from quantities (see details in the green book

https://iupac.org/projects/project-details/?project\_nr=110-2-81 or http://www.sbq.org.br/livroverde/):

For graphs, use slashes in X and Y axes to separate axes names from units. For example:  $2\theta$  / degree; Temperature /  $^{\circ}$ C; time / min; Size range / mm; Wavenumber / cm  $^{-1}$ . Use parentheses only to group a set of units, e.g., Concentration / (mol L  $^{-1}$ );  $10^{3}$  (T/K)  $^{-1}$ , etc.

Pay close attention to the way decimal values are expressed in English. Employ dots instead of commas.

**Figures** must have a high quality in order to be well reproduced. Use at least a 900 dpi resolution. If necessary, resize to a smaller size to get higher quality.

Curves should be labeled (a), (b), (c) etc. and further information be given in the figure legend/caption.

**Data Points** must be shown sufficiently large to be distinguishable. Whenever possible, they should be marked with the following symbols (use alternated full and open symbols):

$$\bullet$$
,  $\circ$ ,  $\blacksquare$ ,  $\Box$ ,  $\triangle$ ,  $\Delta$ ,  $\blacklozenge$ ,  $\Diamond$ 

**Graphs/Figures** should be pasted from their original files (Origin, ChemDraw, Corel etc.) and have an excellent quality. If you have to digitalize (scan) the figures (photos, for instance), choose the following scan options: black & white (B&W), no background and minimum of 300 dpi. If you wish them to be published online in color, send both the colored and B&W versions to the Editorial Office, matching the captions of the figures to accommodate the alternatives.

For computer-generated artwork, background or shadings should be avoided.

# 4.2 Structural Formulae

Figures, schemes and structures should be drawn to fit single or double-column widths. They should look proportional in case they are reduced.

Structures should be numbered with bold Arabic numerals, e.g., 1, 2.

All chemical structures included in the manuscript should be drawn using the same letter type (Times New Roman or Arial), size of cyclic groups, size and thickness of chemical bonds, and, the most important, authors should use the same standard throughout the work, including all figures, schemes, etc.

The following organic group abbreviations may be used: Me, Et, <sup>n</sup>Pr, <sup>n</sup>Bu, <sup>s</sup>Bu, <sup>t</sup>Bu, Ph, CO <sup>2</sup>R, CO <sup>2</sup>H, <sup>i</sup>PrOH.

One variable univalent substituent is indicated by R. When more than one independent variable general substituent is present,  $R^{-1}$ ,  $R^{-2}$ ,  $R^{-3}$ , etc. should be used.

A variable metal may be indicated by M and variable ligands by L<sup>1</sup>, L<sup>2</sup>, L<sup>3</sup> or L1, L2, L3, etc.

# 4.3 Photographs

Photographs should be highly contrasted, positive and not mounted.

When necessary, the scale should be drawn on the photograph itself and not below.

Color prints are rarely reproduced satisfactorily in black and white. Original B&W photographs are preferred to report experimental results, such as electron micrographs or to illustrate special equipment adaptations.

# 4.4 Tables, Data and Units

#### **Tables**

Format your table to give straightforward information to the reader. Do not use shades or bold lettering. Indicate any extra information as a footnote with letters, e.g., a, b, c, etc. For examples, see any "PDF" files in: http://jbcs.sbq.org.br/forthcoming\_papers.asp.

# Data

For negative numbers, ions and equations in text and tables use – (negative symbol) instead of - (hyphen). Examples: Cl  $^-$ , -0.40, y = a x - b.

#### Units

Use International System Units (SI), e.g., m, s, kg, Pa, mol L<sup>-1</sup>, etc, separated from quantities with a blank space. Example: 300 K, not 300K. See: https://iupac.org/what-we-do/books/color-books/.

**Note**: IUPAC convention recommends to avoid the unit Molar (M), being suggested mol L <sup>-1</sup> or mol dm <sup>-3</sup>, with consistent use throughout your manuscript.

For examples, see any "PDF" files in: http://jbcs.sbq.org.br/forthcoming\_papers.asp

# 5. Graphical Abstract (GA) and Text for GA

Concerning the *JBCS* Table of Contents, it is expected from authors careful with their **Graphical Abstract** (**GA**) proposition. This image is the one used in the JBCS posts in the social media (Facebook and Instagram) and index, so it is very important to propose a creative figure summarizing the work, and <u>the resolution is fundamental</u>.

This way, the figure should summarize the content of the manuscript in a <u>concise</u>, <u>pictorial form</u>, <u>designed to capture</u> the attention of a wide readership. The author should present a new figure, using as an idea a key structure, a reaction, an equation, a concept, a graphic, a theorem, etc. It should be used colors as much as possible and have an <u>artistic and imaginative idea</u>. Short movies are also welcome (as supplementary information (SI)). It is not acceptable photos of commercial equipment in GA or in the text of the manuscripts.

**Pay Attention:** the image should have a 900 dpi resolution (\*.tiff / \*.jpg or any other image file that can be edited and be 8 cm wide and 4 cm high). Along with the GA figure, insert a short explanatory text about it below (three lines at the most).

Take a look at our recent publications whose Table of Contents presents Graphical Abstracts (http://jbcs.sbq.org.br). Therefore, be smart to advertise your manuscript, send a beautiful and appealing graphical image.

# 6. Equations

When writing equations, use the Word editing equation option or any other equation editor. Equation cannot be added in the main text as image format.

# 7. How to Cite a Reference throughout the Text

Citations should be typed just after punctuation (without space) as superscripts, see the example:

```
example 1: ... of the environment. 1-8 A behavior... {1-8 as superscripts}
INSTEAD OF: ... of the environment, <sup>1-8</sup>. A behavior... {1-8 as superscripts}
INSTEAD OF: ... of the environment. <sup>1-8</sup> A behavior... {1-8 as superscripts}
```

#### 8. References

Authors are responsible for the accuracy and completeness of all references.

- -> Attention to punctuations ",", ";", ".", and upper and lowercases, and upper and lowercases they are also important in the format of references.
- -> Numbering format of the reference list is in arabic followed by dot:
- 1.
- 2.

# (i) General rules

- (i.a) There should be a space between author name initials: "... AuthorFamilyName, C. F. D. ..." (C. F. D. with space)
- (i.b) There should be a semicolon (;) before journal abbreviation (...W.; Aquino, B. F.; Eng. San. Amb. ...)
- (i.c) There should be a semicolon (;) between the author names (...W.; Aquino, B. F.; Eng. San. Amb. ...)
- (i.d) There should be a comma (,) between Authorfamilyname and initials (...W.; Aquino, B. F.; Eng. ...)
- (i.e) There should <u>not</u> be comma (,) <u>after the periodic name</u>
- (i.f) There should not be fascicle information "...J. Mater. Chem. 1995, 5(2), 331."
- (*i.g*) DOI URL should be included after the page "...117241. [https://doi.org/10.1016/j.jlumin.2020.117241]" (*i.h*) There should not be comma the word "et al.", informe the complete list of the author names

Carefully see how to add the author names: ex. "Liu, W.; Liang Cheng, L.; Xinding Yao, X.;..." ex. "Silva, M. P.; Pereira, X. M.;..."

# (ii) Citing articles

The JBCS rules for reference citation list must be strictly followed.

Mendeley Desktop users can download the citation style for articles in the option ("More styles" -> "Get more Styles") using the following link: http://csl.mendeley.com/styles/242715311/JBCS-3

Mendeley Reference Manager/Mendeley Cite users can download the citation style <u>for articles</u> in the option ("Citation Settings" -> "Change Citation Styles"-> "Add a custom style"-> insert the following link http://csl.mendeley.com/styles/242715311/JBCS-3 -> "Update citation style".

- -> Check periodic abbreviations at https://www.cas.org/content/references/corejournals.
- -> Pay attention in dot for periodic abbreviations: Comput. Math. Methods Med. INSTEAD OF Comput Math Methods Med

The style for article citation is as follows:

Article

- 1. Authorfamilyname1,... A. C. R.; Authorfamilyname2, B.; *J. Braz. Chem. Soc. (italic font)* **2010** (**bold font**), *21 (italic font)*, 77 (just the initial page). [DOI URL]
- 1. Macrino, C. J.; Borges, A. S.; Cunha Neto, A.; Lacerda Jr., V.; Romão, W.; *J. Braz. Chem. Soc.* **2022**, *33*, 173. [https://dx.doi.org/10.21577/0103-5053.20210134]
- 2. Sun, Y.; Li, Q.; Wei, S.; Zhao, R.; Han, J.; Ping, G.; *J. Lumin.* **2020**, 225, 117241. [https://doi.org/10.1016/j.jlumin.2020.117241]

In case the journal is not easily accessible, the best choice is to quote its Chemical Abstracts number, as follows:

3. Provstyanoi, M. V.; Logachev, E. V.; Kochergin, P. M.; Beilis, Y. I.; *Izv. Vyssh. Uchebn. Zadev.; Khim. Khim. Tekhnol.* **1976**, *19*, 708 (*CA* 85:78051s).

Attention to the connection words in the names, as for instance: da Silva, M. A. or Silva, M. da, as follows:

4. Guarieiro, A. L. N.; Eiguren-Fernandez, A.; da Rocha, G. O.; de Andrade, J. B.; *J. Braz. Chem. Soc.* **2017**, 8, 1351. [https://dx.doi.org/10.21577/0103-5053.20210046]

# (iii) Citing books

The style for book citation is as follows:

Book

- 5. Authorfamilyname1,... J.; Authorfamilyname2, M.; *Electron Microscopy (Book title in italic font)*, vol. 1, 2<sup>nd</sup> ed.; Elsevier: London, UK, 1992. [in case of electronic address to access the book, the link should be informed]
- -> [...; Publisher: City, Country, publication year.]
- 5. Regitz, M. In *Multiple Bonds and Low Coordination in Phosphorus Chemistry*; Regitz, M.; Scherer, O. J., eds.; Georg Thieme Verlag: Stuttgart, Germany, 1990, ch. 2.

Book with editor's name

6. Authorfamilyname1,... C. T.; Authorfamilyname2, W. In *Infrared Spectroscopy* editor's name (*Book title in italic font*), vol. 2, 3<sup>rd</sup> ed.; Editorfamilyname1, T. V.; Editorfamilyname2, C. W., eds.;

Elsevier: London, UK, 1992. [in case of electronic address to access the book, the link should be informed]

- -> [...; Publisher: City, Country, publication year.]
- 6. Tsutsumi,... L. H.; Oishi, D. E. In *Specialty Crops for Pacific Island Agroforestry*; Elevitch, C. R., ed; Permanent Agriculture Resources: Holualoa, USA, 2010.

[https://hilo.hawaii.edu/academics/cafnrm/faculty/documents/Tsutsumi-HoneyBeesProfile.pdf] accessed in January 2022

# (iv) Citing software

Software/program (employed in the investigation) should be included in the reference list. Cite the developer instead of publication that used the software (although both can be cited, being that the developer citation is mandatory).

Developer; Software's name (in italic), version; Company/University/etc., Country, year.

- 7. Rasband, W.; ImageJ, 2.0.0-rc-3; National Institutes of Health, USA, 2014.
- 8. Santa-Cruz, P. A.; Teles, F. S.; *Spectra Lux Software* v.2.0 Beta; Ponto Quântico Nanodispositivos/RENAMI, Brasil, 2003.
- 9. Matlab®, version 7b; The MathWorks Inc.; Natick, MA, USA, 2007.

# (v) Citing web addresses

Give preference in citing indexed publication instead of citing websites. For website citation, **title**, **URL** and its **day of access** should be informed, like the example:

Move electronic addresses (like <a href="https://genoma.ib.usp.br/en">https://genoma.ib.usp.br/en</a>) to the reference list, add date of access, and reorganize reference citation.

10. Sociedade Brasileira de Química, <a href="http://www.sbq.org.br">http://www.sbq.org.br</a>, accessed in January 2022.

# (vi) Citing Dissertation/Thesis

This is only accepted as bibliographic reference if available online, the terms "MSc Dissertation" and "PhD Thesis" should be informed, as follows:

11. Frin, K. P. M.: *Propriedades Fotoquímicas de alguns Complexos de Ferro(II) e Rênio(I)*; PhD Thesis, University of São Paulo, São Paulo, Brazil, 2008.

 $[\underline{https://www.teses.usp.br/teses/disponiveis/46/46134/tde-17052016-143939}/pt-br.php]$ 

# (vii) Composite references

They should be used whenever possible, rather than a series of individual references, without letters (a), (b), (c), etc. Use only a semi-colon to separate them. The style for composite references is as follows:

12. Knapp, R. R.; Tona, V.; Okada, T.; Sarpong, R.; Garg, N. K.; *Org. Lett.* **2020**, *22*, 8430 [https://doi.org/10.1021/acs.orglett.0c03052]; Adamo, C. B.; Junger, A. S.; Jesus, D. P.; *Quim. Nova* 

**2021**, *44*, 1360 [http://dx.doi.org/10.21577/0100-4042.20170782]; Kefeni, K. K.; Mamba, B. B.; *Sustainable Mater. Technol.* **2020**, *23*, 140 [https://doi.org/10.1016/j.susmat.2019.e00140].

# (viii) Citing patents

They should be identified in the following form. Whenever possible, Chemical Abstracts numbers should be quoted in parentheses, check the following example:

- 13. Stugess, M. A.; Yand, K.; US pat. 20030232801A1, 2003.
- 14. Kadin, S. B.; US pat. 4,730,004 **1988** (CA 110:P23729y).

# (ix) Citing preprints

The preprint DOI (link) needs to be cited in the reference list of the submitted manuscript, the style is as follows:

15. Neves, B. J.; Moreira-Filho, J. T.; Silva, A. C.; Borba, J. V. V. B.; Mottin, M.; Alves, V. M.; Braga, R. C.; Muratov, E. N.; Andrade, C. H.; *ChemRxiv*, 2020.

[https://chemrxiv.org/articles/preprint/Automated\_Framework\_for\_Developing\_Predictive\_Machine\_Learning\_Models\_for\_Data-Driven\_Drug\_Discovery/12250046/1] accessed in July 2020

# (x) Unpublished material reference

For material **accepted** for publication: <u>in this case</u>, <u>the DOI number should be provided by the authors.</u> For other reference examples, see "PDF" files in: http://jbcs.sbq.org.br/forthcoming\_papers.

16. Valderrama, L.; Demczuk Jr., B.; Valderrama, P; Carasek, E.; *J. Braz. Chem. Soc.*, DOI 10.21577/0103-5053.20210153.

# Other examples for specific documents

- 17. Conselho Nacional do Meio Ambiente (CONAMA); Resolução No. 491, de 19 de novembro de 2018, Dispõe sobre *Padrões de Qualidade do Ar*; Diário Oficial da União (DOU), Brasília, No. 223, de 21/11/2018, p. 155. [https://www.in.gov.br/web/guest/materia/-/asset\_publisher/Kujrw0TZC2Mb/content/id/51058895/do1-2018-11-21-resolucao-n-491-de-19-de-novembro-de-2018-51058603] accessed in September 2021
- 18. Agência Nacional do Petróleo, Gás Natural e Biocombustíveis (ANP); *Anuário Estatístico Brasileiro do Petróleo, Gás Natural e Biocombustíveis*; ANP: Rio de Janeiro, 2018. [https://www.gov.br/anp/pt-br/centrais-de-conteudo/publicacoes/anuario-estatistico/arquivos-anuario-estatistico-2018/anuario 2018.pdf] accessed in September 2021
- 19. Agência Nacional de Vigilância Sanitária (ANVISA); Resolução da Diretoria Colegiada (RDC) No. 239, de 26 de julho de 2018, *Estabelece os Aditivos Alimentares e Coadjuvantes de Tecnologia Autorizados para Uso em Suplementos Alimentares*; Diário Oficial da União (DOU), Brasília, No. 144, de 27/07/2018, p. 90.

[https://www.in.gov.br/materia/-/ asset\_publisher/Kujrw0TZC2Mb/content/id/34380515/do1- 2018-07-27-resolucao-da-diretoria-colegiada-rdc-n-239-de26-de-julho-de-2018-34380387] accessed in September 2021

- 20. Presidência da República Casa Civil; Lei No. 11.097, de 13 de janeiro de 2005, Dispõe sobre a *Introdução do Biodiesel na Matriz Energética Brasileira*; Diário Oficial da União (DOU), Brasília, Brazil, 2005. [https://www.planalto.gov.br/ccivil 03/ ato2004-2006/2005/lei/11097.htm] accessed in November 2021
- 21. Commission of the European Communities; 488/2014/ EC: Commission Decision of 12 May 2014; Official Journal of the European Union, 2014, L 138, p. 75. [https://eur-lex.europa.eu/legal-content/en/
  TXT/?uri=CELEX%3A32014R0488] accessed in September 2021
- 22. United States Environmental Protection Agency (US EPA); *Method IO-3.4: Determination of Metals in Ambient Particulate Matter Using Inductively Coupled Plasma (ICP) Spectroscopy*; US EPA: Cincinnati, 1999. [ <a href="https://www.epa.gov/sites/default/files/2015-07/documents/epa-io-3.4.pdf">https://www.epa.gov/sites/default/files/2015-07/documents/epa-io-3.4.pdf</a>] accessed in December 2021
- 23. World Health Organization (WHO); Environmental Health Criteria 239, Principles for Modelling Dose-Response for the Risk Assessment of Chemicals; WHO: Geneva, Switzerland, 2009. [https://apps.who.int/iris/handle/10665/43940] accessed in December 2019
- 24. ISO Guide 35: Reference Materials: General and Statistical Principles for Certification, ISO: Geneva, 2006.
- 25. ASTM D664: Standard Test Method for Acid Number of Petroleum Products by Potentiometric Titration, Philadelphia, 2009.
- 26. EN 14104: Fat and Oil Derivatives Fatty Acid Methyl Esters (FAME), Determination of Acid Value, European Committee for Standardization: Berlin, 2003.
- 27. Companhia Ambiental do Estado de São Paulo (CETESB); *Guia Nacional de Coleta e Preservação de Amostras*; CETESB: São Paulo, 2011.
- 28. *The United States Pharmacopoeia (USP)*, USP 37-NF 32, vol. 2, The United States Pharmacopeial Convention, Rockville, 2013, p. 1954-1955.
- 29. British Pharmacopoeia 2019, vol. 1, The Stationery Office, London, 2019, p. I-292-I-293.
- 30. American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE); *Ventilation for Acceptable Indoor Air Quality*, Standard 62-1999, ASHRAE, Inc.: Atlanta, 1999.

- 31. Farmacopeia Brasileira, 4th ed.; Atheneu: São Paulo, 2002.
- 32. International Conference on Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use (ICH); *Validation of Analytical Procedures: Text and Methodology Q2(R1)*; ICH: London, 2005.

For CRM, NIST, AOCS Official/Standard method, ICSD, JCPDS, PDB, Web of Science, Scopus and PubChem, SciFinder and ChemSpider, it is not necessary to include in the reference list.

# 9. Supplementary Information (SI)

This material will be available online in the *JBCS* Page as PDF file. It should contain relevant and complementary data to those presented in the manuscript. Their format can be: tables, graphs, spectra, films and so on.

Any synthesized or identified compound must be accompanied by the spectra used for such identification. This is especially important for Natural Products, Organic and Inorganic Chemistry manuscripts in which the characterization/identification techniques are part of the work.

# 9.1. Manuscripts including crystallographic data

# **Deposition of Crystallographic Data**

Prior to the submission of the typescript including crystallographic data, the author(s) should deposit, in the relevant Data Center, the data corresponding to each structure to be reported.

Data for **organometallic, organic, coordination (Werner-type) and inorganic compounds** should be sent to the joint CCDC/FIZ Karlsruhe online deposition service (<a href="https://www.ccdc.cam.ac.uk/Community/depositastructure/">https://www.ccdc.cam.ac.uk/Community/depositastructure/</a>), in CIF format. More information about the deposit can be obtained from the CCDC/FIZ Frequently Asked Questions (FAQ) homepage: <a href="https://www.ccdc.cam.ac.uk/support-and-resources/Support/search?c=d738a58f-c4ab-49f3-95af-569f2fe5d2f9">https://www.ccdc.cam.ac.uk/support-and-resources/Support/search?c=d738a58f-c4ab-49f3-95af-569f2fe5d2f9</a>.

CCDC: Cambridge Crystallographic Data Centre (<a href="https://www.ccdc.cam.ac.uk/">https://www.ccdc.cam.ac.uk/</a>) FIZ: Fachinformationszentrum (<a href="https://www.fiz-karlsruhe.de/">https://www.fiz-karlsruhe.de/</a>).

# **Deposition Codes**

The Data Centers will provide deposition codes for each data set, which should be quoted in the typescript under a Supplementary Information heading before the Acknowledgements.

Standard text for CCDC:

Crystallographic data (excluding structure factors) for the structures in this work were deposited in the Cambridge Crystallographic Data Centre as supplementary publication number CCDC XXXXXX. Copies of the data can be obtained, free of charge, via <a href="https://www.ccdc.cam.ac.uk/structures/">https://www.ccdc.cam.ac.uk/structures/</a>.

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During submission of a manuscript to the *Journal of the Brazilian Chemical Society*, authors should provide CCDC/FIZ reference numbers as Supplementary Information according to the instructions given above. CIF files should not be submitted with the manuscript (only to the suitable Data Center). Any revised CIF generated during the editorial process should be deposited directly with the CCDC before the revised manuscript is submitted to the JBCS.

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# **Preparation of Crystallographic Material**

When the manuscript is submitted, the following guidelines should be observed:

The Abstract should not contain crystal data, but a concise statement of the main features of the structural results.

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- 9.1.1 Color, habit and size of the crystal(s) used, behavior of the compound under the data collection conditions.
- 9.1.2 The chemical formula should correspond to the complete chemical unit encompassing the crystallographic symmetry, the formula weight, F(000), the absorption coefficient and the measured and calculated densities.
- 9.1.3 The unit cell parameters with esd's and the X-ray wavelength used.
- 9.1.4 The crystal system, space group and number of chemical units *per* cell.
- 9.1.5 Type of diffractometer used and method of data collection, total number of data collected, number of unique reflections, R(int) value, number of observed reflections with cut-off parameter, use or not of absorption correction, transmission factors.
- 9.1.6 The final results: R, wR, S and the number of parameters refined; treatment of hydrogen atoms; final peak and hole in the last difference map. Only refinements on F2 will be accepted.

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It must include a labeled diagram of the structure, a list of relevant geometric parameters - interatomic bond distances and angles, torsion angles, hydrogen bond parameters, etc. Data of less important parts of the structure, such as ligand sub-groups (phenyl rings, etc.) should be omitted.

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Whenever a compound is synthesized or identified (new or already known), it is imperative to send all spectral data (data and spectra) as Supplementary Information (SI) along with your submission, at the end of your doc file.

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