DESCRIPTION

The Journal of Chemical Thermodynamics exists primarily for dissemination of significant new knowledge in experimental equilibrium thermodynamics and transport properties of chemical systems. The defining attributes of The Journal are the quality and relevance of the papers published.

The Journal publishes work relating to gases, liquids, solids, polymers, mixtures, solutions and interfaces. Studies on systems with variability, such as biological or bio-based materials, gas hydrates, among others, will also be considered provided these are well characterized and reproducible where possible. Experimental methods should be described in sufficient detail to allow critical assessment of the accuracy claimed.

Authors are encouraged to provide physical or chemical interpretations of the results. Articles can contain modelling sections providing representations of data or molecular insights into the properties or transformations studied. Theoretical papers on chemical thermodynamics using molecular theory or modelling are also considered.

The Journal welcomes review articles in the field of chemical thermodynamics but prospective authors should first consult one of the Editors concerning the suitability of the proposed review.

Contributions of a routine nature or reporting on uncharacterised materials are not accepted.

We strongly encourage all authors to use EES at the following URL when submitting papers to The Journal of Chemical Thermodynamics.

EES can be accessed at: http://ees.elsevier.com/jct
(First time users will need to register)

622860jct.gif

JCT Style guide
Please consult the Guide for Authors for further details on the requirements for submitting your paper to The Journal of Chemical Thermodynamics. The guidelines described in this document, as well as those listed in the JCT Style Notes, should be carefully adhered to ensure high-quality and rapid publication of your manuscript.
IMPACT FACTOR

2018: 2.290 © Clarivate Analytics Journal Citation Reports 2019

ABSTRACTING AND INDEXING

Scopus
ASCA
Chem Inform
Chemical Abstracts
Chemical Titles
Chemistry Citation Index
Current Contents - Physical, Chemical & Earth Sciences
Engineered Materials Abstracts
Physics Abstracts
Reaction Citation Index
Research Alert
Science Citation Index
INSPEC

EDITORIAL BOARD

Editors
W.E. Acree, Jr., University of North Texas Department of Chemistry, NT Station, Box 305070, Denton, Texas, 76203-5017, United States
R. Weir, Royal Military College Of Canada Department of Chemistry and Chemical Engineering, PO Box 17000 STN Forces, Kingston, K7K 7B4, Ontario, Canada

Advisory Board
M. Anouti, Tours, France
M. Bastos, Porto, Portugal
A. Bazyleva, Boulder, CO, USA
J.G. Beltran, Kingston, Ontario, Canada
M. Bendova, Prague, Czech Republic
J. Chickos, Saint Louis, Missouri, United States
S. Choudhary, Mumbai, India
M. Costas, Mexico, Mexico
P.T. Cummings, Nashville, Tennessee, United States
S. Dasgupta
U. Deiters, Cologne, Germany
U. Domańska-Żelazna, Warsaw, Poland
M. Dzida, Katowice, Poland
R. Fernandez-Prini, Buenos Aires, Argentina
L.A. Galicia-Luna, Ciudad de Mexico, Mexico
S. Hamzehzadeh, Tehran, Iran, Islamic Republic of
B. Han, Beijing, China
M. He, Xi’an, China
T.P. Iglesias, Ourense, Spain
A. Jouyban, Tabriz, Iran, Islamic Republic of
M. Kljevcancin, Belgrade, Serbia
H. Kim, Seoul, Korea, Republic of
N. Kishore, Mumbai, India
M.C. Kroon, Abu Dhabi, United Arab Emirates
I. Lampireia, Lisboa, Portugal
T.M. Letcher, Stratton On The Fosse Bath, Radstock, United Kingdom
J.F. Liebman, Baltimore, Maryland, United States
Y. Liu, Wuhan, China
W. Loh, Campinas, São Paulo, Brazil
R. Majdan-Cegincara, Tehran, Iran, Islamic Republic of
F. Martinez Rodriguez, Bogotá D.C, Colombia
N.I. Matskevich, Novosibirsk, Russian Federation
M.E. Minas de Piedad, Lisboa, Portugal
M.J.S. Monte, Porto, Portugal
F. Mutelet, Vandœuvre-lès-Nancy, France
A.K. Nain, New Delhi, India
A. Navrotsky, Davis, California, United States
A. Patnaik, Chennai, India
P. Pendelton, Adelaide, South Australia, Australia
G. Perlovich, Ivanovo, Russian Federation
D. Ramjugernath, Durban, South Africa
A.C.F Ribeiro, Coimbra, Portugal
M.D.M.C. Ribeiro da Silva, Porto, Portugal
A. Rodriguez, Vigo, Spain
K. Ruzicka, Praha, Czech Republic
K. Saito, Tsukuba, Japan
B. Shiflett, Lawrence, Kansas, United States
W. Su, Tianjin, China
L.-X. Sun, Dalian, China
K. Tamura, Kanazawa, Japan
Z.-C Tan, Dalian, China
J. Troncoso, Ourense, Spain
J.P.M. Trusler, London, United Kingdom
P. Venkatesu, New Delhi, India
S.P. Verevkin, Rostock, Germany
W.A. Wakeham, Southampton, United Kingdom
J. Wang, Xinyang, China
Y. Wang, Beijing, China
B.F. Woodfield, Provo, Utah, United States
M.T. Zafarani-Moattar, Tabriz, Iran, Islamic Republic of
J. Zhang, Beijing, China
Your Paper Your Way
We now differentiate between the requirements for new and revised submissions. You may choose to submit your manuscript as a single Word or PDF file to be used in the refereeing process. Only when your paper is at the revision stage, will you be requested to put your paper in to a 'correct format' for acceptance and provide the items required for the publication of your article.
To find out more, please visit the Preparation section below.

INTRODUCTION

General
Please consult this Guide for Authors for further details on the requirements for submitting your paper to The Journal of Chemical Thermodynamics. The guidelines described in this document, as well as those listed in the JCT Style Notes, should be carefully adhered to ensure high-quality and rapid publication of your manuscript.

Aims and Scope
The Journal of Chemical Thermodynamics exists primarily for dissemination of significant new measurements in experimental thermodynamics and thermophysics including bio-thermodynamics, calorimetry, phase equilibria, equilibrium thermodynamic properties and transport properties.

The Journal publishes work relating to gases, liquids, solids, mixtures, solutions, interfaces, including polymers and biological materials, provided that the systems studied are characterised and reproducible.

The defining attributes of The Journal are the quality and relevance of the papers published. Authors are expected to describe their methods and present their results in sufficient detail to allow critical assessment of the accuracy claimed.

Further, The Journal welcomes theoretical papers reporting on thermodynamics using molecular theory or modeling, provided the relationship with experiment is clearly described. Review articles will also be considered but prospective authors should first consult one of the Editors concerning the suitability of the proposed review.

Experimental measurements of a routine nature or those conducted on uncharacterised materials are not accepted.

The Journal of Chemical Thermodynamics, along with other journals in the field, cooperates with the Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST) for the purpose of ensuring the quality of published experimental data. This collaboration relates to articles that report experimental measurements falling within the scope of the NIST ThermoML Archive (http://www.trc.nist.gov/ThermoML.html) and has two elements. First, upon submission of an article, NIST will provide a literature report to the authors and reviewers containing relevant references from the NIST Data Archive. Second, NIST will provide a data evaluation at the end of the review process immediately prior to acceptance of the article. This data evaluation will compare the reported experimental data with that existing in the NIST Data Archive and highlight any unexpectedly large discrepancies such as those arising from typographical errors. In order to facilitate the necessary electronic data capture, the experimental results and their uncertainties must be tabulated as described in this Guide (see also http://trc.nist.gov/JCT-Support.html).
For more information, please read the Editorial

Submission checklist
You can use this list to carry out a final check of your submission before you send it to the journal for review. Please check the relevant section in this Guide for Authors for more details.

Ensure that the following items are present:

One author has been designated as the corresponding author with contact details:
• E-mail address
• Full postal address
All necessary files have been uploaded:

**Manuscript:**
- Include keywords
- All figures (include relevant captions)
- All tables (including titles, description, footnotes)
- Ensure all figure and table citations in the text match the files provided
- Indicate clearly if color should be used for any figures in print

**Graphical Abstracts / Highlights files** (where applicable)

**Supplemental files** (where applicable)

**Further considerations**
- Manuscript has been 'spell checked' and 'grammar checked'
- All references mentioned in the Reference List are cited in the text, and vice versa
- Permission has been obtained for use of copyrighted material from other sources (including the Internet)
- A competing interests statement is provided, even if the authors have no competing interests to declare
- Journal policies detailed in this guide have been reviewed
- Referee suggestions and contact details provided, based on journal requirements

For further information, visit our [Support Center](http://www.elsevier.com/locate/jct).

**BEFORE YOU BEGIN**

**Ethics in publishing**
Please see our information pages on [Ethics in publishing](http://www.elsevier.com/locate/jct) and [Ethical guidelines for journal publication](http://www.elsevier.com/locate/jct).

**Declaration of interest**
All authors must disclose any financial and personal relationships with other people or organizations that could inappropriately influence (bias) their work. Examples of potential conflicts of interest include employment, consultancies, stock ownership, honoraria, paid expert testimony, patent applications/registrations, and grants or other funding. Authors should complete the declaration of interest statement using [this template](http://www.elsevier.com/locate/jct) and upload to the submission system at the Attach/Upload Files step. If there are no interests to declare, please choose: 'Declarations of interest: none' in the template. This statement will be published within the article if accepted. [More information](http://www.elsevier.com/locate/jct).

**Submission declaration and verification**
Submission of an article implies that the work described has not been published previously (except in the form of an abstract, a published lecture or academic thesis, see 'Multiple, redundant or concurrent publication' for more information), that it is not under consideration for publication elsewhere, that its publication is approved by all authors and tacitly or explicitly by the responsible authorities where the work was carried out, and that, if accepted, it will not be published elsewhere in the same form, in English or in any other language, including electronically without the written consent of the copyright-holder. To verify originality, your article may be checked by the originality detection service Crossref Similarity Check.

**Preprints**
Please note that preprints can be shared anywhere at any time, in line with Elsevier's [sharing policy](http://www.elsevier.com/locate/jct). Sharing your preprints e.g. on a preprint server will not count as prior publication (see 'Multiple, redundant or concurrent publication' for more information).

**Use of inclusive language**
Inclusive language acknowledges diversity, conveys respect to all people, is sensitive to differences, and promotes equal opportunities. Articles should make no assumptions about the beliefs or commitments of any reader, should contain nothing which might imply that one individual is superior to another on the grounds of race, sex, culture or any other characteristic, and should use inclusive language throughout. Authors should ensure that writing is free from bias, for instance by using 'he or she', 'his/her' instead of 'he' or 'his', and by making use of job titles that are free of stereotyping (e.g. 'chairperson' instead of 'chairman' and 'flight attendant' instead of 'stewardess').
Author contributions
For transparency, we encourage authors to submit an author statement file outlining their individual contributions to the paper using the relevant CRediT roles: Conceptualization; Data curation; Formal analysis; Funding acquisition; Investigation; Methodology; Project administration; Resources; Software; Supervision; Validation; Visualization; Roles/Writing - original draft; Writing - review & editing. Authorship statements should be formatted with the names of authors first and CRediT role(s) following. More details and an example

Changes to authorship
Authors are expected to consider carefully the list and order of authors before submitting their manuscript and provide the definitive list of authors at the time of the original submission. Any addition, deletion or rearrangement of author names in the authorship list should be made only before the manuscript has been accepted and only if approved by the journal Editor. To request such a change, the Editor must receive the following from the corresponding author: (a) the reason for the change in author list and (b) written confirmation (e-mail, letter) from all authors that they agree with the addition, removal or rearrangement. In the case of addition or removal of authors, this includes confirmation from the author being added or removed.
Only in exceptional circumstances will the Editor consider the addition, deletion or rearrangement of authors after the manuscript has been accepted. While the Editor considers the request, publication of the manuscript will be suspended. If the manuscript has already been published in an online issue, any requests approved by the Editor will result in a corrigendum.

Copyright
Upon acceptance of an article, authors will be asked to complete a 'Journal Publishing Agreement' (see more information on this). An e-mail will be sent to the corresponding author confirming receipt of the manuscript together with a 'Journal Publishing Agreement' form or a link to the online version of this agreement.

Subscribers may reproduce tables of contents or prepare lists of articles including abstracts for internal circulation within their institutions. Permission of the Publisher is required for resale or distribution outside the institution and for all other derivative works, including compilations and translations. If excerpts from other copyrighted works are included, the author(s) must obtain written permission from the copyright owners and credit the source(s) in the article. Elsevier has preprinted forms for use by authors in these cases.

For gold open access articles: Upon acceptance of an article, authors will be asked to complete an 'Exclusive License Agreement' (more information). Permitted third party reuse of gold open access articles is determined by the author's choice of user license.

Author rights
As an author you (or your employer or institution) have certain rights to reuse your work. More information.

Elsevier supports responsible sharing
Find out how you can share your research published in Elsevier journals.

Role of the funding source
You are requested to identify who provided financial support for the conduct of the research and/or preparation of the article and to briefly describe the role of the sponsor(s), if any, in study design; in the collection, analysis and interpretation of data; in the writing of the report; and in the decision to submit the article for publication. If the funding source(s) had no such involvement then this should be stated.

Open access
Please visit our Open Access page from the Journal Homepage for more information.

Elsevier Researcher Academy
Researcher Academy is a free e-learning platform designed to support early and mid-career researchers throughout their research journey. The "Learn" environment at Researcher Academy offers several interactive modules, webinars, downloadable guides and resources to guide you through the process of writing for research and going through peer review. Feel free to use these free resources to improve your submission and navigate the publication process with ease.
Language (usage and editing services)
Please write your text in good English (American or British usage is accepted, but not a mixture of these). Authors who feel their English language manuscript may require editing to eliminate possible grammatical or spelling errors and to conform to correct scientific English may wish to use the English Language Editing service available from Elsevier's Author Services.

Submission
Our online submission system guides you stepwise through the process of entering your article details and uploading your files. The system converts your article files to a single PDF file used in the peer-review process. Editable files (e.g., Word, LaTex) are required to typeset your article for final publication. All correspondence, including notification of the Editor's decision and requests for revision, is sent by e-mail.

Referees
Please submit, with the manuscript, the names and addresses of four potential referees, of which at least two are outside the author's geographical region. It is hoped that this list will be useful during the final checking of an article prior to sending it to the journal's editor for review.

PREPARATION

NEW SUBMISSIONS
Submission to this journal proceeds totally online and you will be guided stepwise through the creation and uploading of your files. The system automatically converts your files to a single PDF file, which is used in the peer-review process.
As part of the Your Paper Your Way service, you may choose to submit your manuscript as a single file to be used in the refereeing process. This can be a PDF file or a Word document, in any format or layout that can be used by referees to evaluate your manuscript. It should contain high enough quality figures for refereeing. If you prefer to do so, you may still provide all or some of the source files at the initial submission. Please note that individual figure files larger than 10 MB must be uploaded separately.

References
There are no strict requirements on reference formatting at submission. References can be in any style or format as long as the style is consistent. Where applicable, author(s) name(s), journal title/book title, chapter title/article title, year of publication, volume number/book chapter and the article number or pagination must be present. Use of DOI is highly encouraged. The reference style used by the journal will be applied to the accepted article by Elsevier at the proof stage. Note that missing data will be highlighted at proof stage for the author to correct.

Formatting requirements
There are no strict formatting requirements but all manuscripts must contain the essential elements needed to convey your manuscript, for example Abstract, Keywords, Introduction, Materials and Methods, Results, Conclusions, Artwork and Tables with Captions.
If your article includes any Videos and/or other Supplementary material, this should be included in your initial submission for peer review purposes.
Divide the article into clearly defined sections.

Figures and tables embedded in text
Please ensure the figures and the tables included in the single file are placed next to the relevant text in the manuscript, rather than at the bottom or the top of the file. The corresponding caption should be placed directly below the figure or table.

Reporting New Experimental Data
Do you report any experimental results in the submission?

Yes.
Before your manuscript reporting new experimental results is submitted to the Journal of Chemical Thermodynamics, your submission should be checked for the items listed Here

Kindly download the checklist and fill it appropriately as per the above instructions. This attachment should be submitted along with the manuscript under the file type "Validation Report"

No.
Stop here - it is only to report experimental data.
**Peer review**
This journal operates a single blind review process. All contributions will be initially assessed by the editor for suitability for the journal. Papers deemed suitable are then typically sent to a minimum of two independent expert reviewers to assess the scientific quality of the paper. The Editor is responsible for the final decision regarding acceptance or rejection of articles. The Editor's decision is final. More information on types of peer review.

**REVISED SUBMISSIONS**

*Use of word processing software*
Regardless of the file format of the original submission, at revision you must provide us with an editable file of the entire article. Both highlighted (marked) and non-highlighted (unmarked/clear) versions of the revised manuscript are required as a part of the final PDF for revision. The highlighted version of the manuscript will have the changes, made during revision, highlighted in a different color to help the editors and reviewers spot these changes easily during the review process. Both highlighted and non-highlighted version of the revised manuscript can be uploaded using the submission item 'Manuscript' in the 'Attach Files' step. This is mandatory for revisions submitted to the journal.

Keep the layout of the text as simple as possible. Most formatting codes will be removed and replaced on processing the article. The electronic text should be prepared in a way very similar to that of conventional manuscripts (see also the Guide to Publishing with Elsevier: https://www.elsevier.com/guidepublication).
See also the section on Electronic artwork.
To avoid unnecessary errors you are strongly advised to use the ‘spell-check’ and ‘grammar-check’ functions of your word processor.

*LaTeX*
You are recommended to use the Elsevier article class elsarticle.cls to prepare your manuscript and BibTeX to generate your bibliography.
Our LaTeX site has detailed submission instructions, templates and other information.

**Article structure**

*Subdivision - numbered sections*
Divide your article into clearly defined and numbered sections. Subsections should be numbered 1.1 (then 1.1.1, 1.1.2, ...), 1.2, etc. (the abstract is not included in section numbering). Use this numbering also for internal cross-referencing: do not just refer to 'the text'. Any subsection may be given a brief heading. Each heading should appear on its own separate line.

*Introduction*
State the objectives of the work and provide an adequate background, avoiding a detailed literature survey or a summary of the results.

*Experimental*
Provide sufficient details to allow the work to be reproduced by an independent researcher. Methods that are already published should be summarized, and indicated by a reference. If quoting directly from a previously published method, use quotation marks and also cite the source. Any modifications to existing methods should also be described.

*Results*
Results should be clear and concise.

*Discussion*
This should explore the significance of the results of the work, not repeat them. A combined Results and Discussion section is often appropriate. Avoid extensive citations and discussion of published literature.

*Conclusions*
The main conclusions of the study may be presented in a short Conclusions section, which may stand alone or form a subsection of a Discussion or Results and Discussion section.

*Appendices*
If there is more than one appendix, they should be identified as A, B, etc. Formulae and equations in appendices should be given separate numbering: Eq. (A.1), Eq. (A.2), etc.; in a subsequent appendix, Eq. (B.1) and so on. Similarly for tables and figures: Table A.1; Fig. A.1, etc.
**Style Requirements**

**Symbols, Units and Equations**

2. SI units should be used throughout.
3. The algebra of quantities must be followed. Accordingly, the symbol for a physical quantity represents a pure number multiplied by a unit or combination of units.
4. Each physical quantity must be represented by a single symbol which may be decorated with subscript or superscript characters.
5. The symbol for a physical quantity must appear in italic or sloping type, even when the symbol appears in a subscript or a superscript. Conversely, symbols not designating a physical quantity should appear in Roman or upright type: e.g. YJCHT_ST_1.JPG represents the perfect-gas molar heat capacity (italic ‘p’ for pressure, Roman ‘m’ for molar).
6. Symbols should be defined in the text when they are first used, and also in figure and table legends.
7. Equations must always be dimensionally consistent. Equations used to correlate experimental data may be best in a dimensionless form.

**Example**

YJCHT_ST_2.JPG

8. The arguments of logarithmic, exponential and trigonometric functions must be dimensionless: e.g. ln(p/MPa) or ln(p/p0) but not ln(p).
9. Equations, when displayed, should be centred and numbered, flush right, in parenthesis eg

YJCHT_ST_3.JPG (1)

10. Always puncture after an equation to place it correctly within the sentence that contains it (see example above).
11. Wherever possible set equation and expressions on a single line: e.g.: dp/dT not YJCHT_ST_4.JPG

**Reporting of Uncertainties**

12. When reporting experimental results, the uncertainty of each measured quantity should be reported and combined in quadrature to obtain the uncertainty of any derived quantities (see http://physics.nist.gov/cuu/).
13. Uncertainties may be specified either as standard uncertainties u or as expanded uncertainties U having a specified confidence interval.

**Figures**

14. Number figures consecutively in accordance with their appearance in the text.
15. Plot each figure in a full rectangular (or triangular) frame.
16. Tick marks should be shown on the lower abscissa and the left ordinate and must project into the plotting area.
17. All lettering to be in 12-point Times Roman or similar typeface.
18. Lettering should be used to specify the scale and axis labels only. All legend material should be provided in a separate figure caption and not shown on the figure itself. Exceptionally, multi-part figures may be labelled (a), (b) etc.
19. Only dimensionless quantities should be plotted. Axis labels must therefore be dimensionless expressions presented in correctly-formatted symbols: e.g. T/K; not T (K) or Temperature/K. All symbols must be defined in the accompanying caption.
20. Fractional deviations and similar quantities should be plotted as, e.g., 10^2(X-X_c)/X_c; do not use ‘ppm’, ‘per cent’, ‘%’ or similar abbreviations.
21. Plotting symbols only should be used to represent experimental data or discretely computed quantities. Smooth lines or curves only should be used to represent values computed from formulae or other continuous data (e.g. g.l.c. trace).
22. Avoid the use of colour in graphs; data sets should be distinguished by symbol or line styles only. Exceptionally, essential colour illustrations may be included.
23. Similar figures should be plotted in identically-sized frames.
24. Triangular diagrams must be equilateral and must have correctly ticked, scaled and labelled axes on all three sides.
25. Include error bars where appropriate but only when they exceed the size of the plotting symbols.
FIGURE 1. (a) Densities $\rho$ of pentafluoroethane at temperatures $T$: , saturated liquid; •, saturated vapour; -------- , saturated vapour and liquid calculated from Eq. (4). (b) Deviations of experimental saturated liquid densities $\rho_1$ from values $\rho_{\text{calc}}$ calculated from Eq. (4).

Tables
26. Number tables consecutively in accordance with their appearance in the text.
27. Tables must be completely self contained with column headings defined fully in the accompanying table legend.
28. Tabulated quantities must be dimensionless. Row and column headings must therefore be dimensionless expressions presented in correctly-formatted symbols: e.g. $T/K$; not $T(K)$ or Temperature/K. All symbols must be defined in the accompanying legend.
29. Footnotes may be cited using lower-case Roman superscripts (e.g. $^{a,b}$). Define the footnotes at the base of the table.
30. The uncertainty of each tabulated quantity must be specified either in a footnote or, if variable, included in the table as an additional column (for further examples, see http://trc.nist.gov/JCT-Support.html).
31. Where experimental values of heat capacities are reported, tabulate the values as, e.g., $C_{p,m}/R$. In addition (but not as an alternative), a column of heat capacity values with units may be given: e.g., $C_p/(J \cdot K \cdot mol^{-1})$.
32. Fractional deviations and similar quantities should be tabulated as, e.g., $10^2(X-X)/X_c$; do not use 'ppm', 'per cent', '%' or similar abbreviations.
33. Missing entries in a table should be shown as blanks.

Miscellaneous
34. All chemical samples must be identified by IUPAC systematic name and the following details should be provided: sample source, initial purity, method of purification, final purity (as used) and analytical method used to determine the purity. Preferably, all of these details should be provided in a table (see http://trc.nist.gov/JCT-Support.html).
35. Purities should be given as mole fraction or mass fractions, e.g. mole fraction 0.99, not 99 mole per cent.
36. Use $p^0$ for the standard pressure and specify its value at first usage.
37. Always insert the name of a quantity or its symbol (but not both) before the value of a quantity: e.g. between the temperatures 298.15 K and 340 K; or between $T = 298.15$ K and $T = 340$ K.
38. Give lists of values as, e.g., $T/K = (300, 400$ and 500) or $T = (300, 400$ or 500) K but not $T = 300, 400$ and $500$ K.
39. Chemical depictions of electrochemical cells should be displayed and numbered with upper case roman numerals.

Essential title page information
• Title. Concise and informative. Titles are often used in information-retrieval systems. Avoid abbreviations and formulae where possible.
• Author names and affiliations. Please clearly indicate the given name(s) and family name(s) of each author and check that all names are accurately spelled. You can add your name between parentheses in your own script behind the English transliteration. Present the authors' affiliation addresses (where the actual work was done) below the names. Indicate all affiliations with a lower-case superscript letter immediately after the author's name and in front of the appropriate address. Provide the full postal address of each affiliation, including the country name and, if available, the e-mail address of each author.
• Corresponding author. Clearly indicate who will handle correspondence at all stages of refereeing and publication, also post-publication. This responsibility includes answering any future queries about Methodology and Materials. **Ensure that the e-mail address is given and that contact details are kept up to date by the corresponding author.**

• Present/permanent address. If an author has moved since the work described in the article was done, or was visiting at the time, a 'Present address' (or 'Permanent address') may be indicated as a footnote to that author's name. The address at which the author actually did the work must be retained as the main, affiliation address. Superscript Arabic numerals are used for such footnotes.

Highlights
Highlights are optional yet highly encouraged for this journal, as they increase the discoverability of your article via search engines. They consist of a short collection of bullet points that capture the novel results of your research as well as new methods that were used during the study (if any). Please have a look at the examples here: example Highlights.

Highlights should be submitted in a separate editable file in the online submission system. Please use 'Highlights' in the file name and include 3 to 5 bullet points (maximum 85 characters, including spaces, per bullet point).

Abstract
A concise and factual abstract is required. The abstract should state briefly the purpose of the research, the principal results and major conclusions. An abstract is often presented separately from the article, so it must be able to stand alone. For this reason, References should be avoided, but if essential, then cite the author(s) and year(s). Also, non-standard or uncommon abbreviations should be avoided, but if essential they must be defined at their first mention in the abstract itself.

Graphical abstract
Although a graphical abstract is optional, its use is encouraged as it draws more attention to the online article. The graphical abstract should summarize the contents of the article in a concise, pictorial form designed to capture the attention of a wide readership. Graphical abstracts should be submitted as a separate file in the online submission system. Image size: Please provide an image with a minimum of 531 × 1328 pixels (h × w) or proportionally more. The image should be readable at a size of 5 × 13 cm using a regular screen resolution of 96 dpi. Preferred file types: TIFF, EPS, PDF or MS Office files. You can view Example Graphical Abstracts on our information site. Authors can make use of Elsevier's Illustration Services to ensure the best presentation of their images and in accordance with all technical requirements.

Highlights
Highlights are mandatory for this journal. They consist of a short collection of bullet points that convey the core findings of the article and should be submitted in a separate file in the online submission system. Please use 'Highlights' in the file name and include 3 to 5 bullet points (maximum 125 characters including spaces, or, maximum 20 words per bullet point). See https://www.elsevier.com/highlights for examples.

Keywords
Immediately after the abstract, provide a maximum of 6 keywords, using British spelling and avoiding general and plural terms and multiple concepts (avoid, for example, 'and', 'of'). Be sparing with abbreviations: only abbreviations firmly established in the field may be eligible. These keywords will be used for indexing purposes.

Abbreviations
Define abbreviations that are not standard in this field in a footnote to be placed on the first page of the article. Such abbreviations that are unavoidable in the abstract must be defined at their first mention there, as well as in the footnote. Ensure consistency of abbreviations throughout the article.

Acknowledgements
Collate acknowledgements in a separate section at the end of the article before the references and do not, therefore, include them on the title page, as a footnote to the title or otherwise. List here those individuals who provided help during the research (e.g., providing language help, writing assistance or proof reading the article, etc.).

Formatting of funding sources
List funding sources in this standard way to facilitate compliance to funder's requirements:
Funding: This work was supported by the National Institutes of Health [grant numbers xxxx, yyyy]; the Bill & Melinda Gates Foundation, Seattle, WA [grant number zzzz]; and the United States Institutes of Peace [grant number aaaa].

It is not necessary to include detailed descriptions on the program or type of grants and awards. When funding is from a block grant or other resources available to a university, college, or other research institution, submit the name of the institute or organization that provided the funding.

If no funding has been provided for the research, please include the following sentence:

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Nomenclature and Units
Follow internationally accepted rules and conventions: use the international system of units (SI). If other quantities are mentioned, give their equivalent in SI.

Footnotes
Footnotes should be used sparingly. Number them consecutively throughout the article. Many word processors build footnotes into the text, and this feature may be used. Should this not be the case, indicate the position of footnotes in the text and present the footnotes themselves separately at the end of the article.

Artwork
Image manipulation
Whilst it is accepted that authors sometimes need to manipulate images for clarity, manipulation for purposes of deception or fraud will be seen as scientific ethical abuse and will be dealt with accordingly. For graphical images, this journal is applying the following policy: no specific feature within an image may be enhanced, obscured, moved, removed, or introduced. Adjustments of brightness, contrast, or color balance are acceptable if and as long as they do not obscure or eliminate any information present in the original. Nonlinear adjustments (e.g. changes to gamma settings) must be disclosed in the figure legend.

Electronic artwork
General points
• Make sure you use uniform lettering and sizing of your original artwork.
• Preferred fonts: Arial (or Helvetica), Times New Roman (or Times), Symbol, Courier.
• Number the illustrations according to their sequence in the text.
• Use a logical naming convention for your artwork files.
• Indicate per figure if it is a single, 1.5 or 2-column fitting image.
• For Word submissions only, you may still provide figures and their captions, and tables within a single file at the revision stage.
• Please note that individual figure files larger than 10 MB must be provided in separate source files.

A detailed guide on electronic artwork is available.

You are urged to visit this site; some excerpts from the detailed information are given here.

Formats
Regardless of the application used, when your electronic artwork is finalized, please 'save as' or convert the images to one of the following formats (note the resolution requirements for line drawings, halftones, and line/halftone combinations given below):

EPS (or PDF): Vector drawings. Embed the font or save the text as 'graphics'.
TIFF (or JJP): Color or grayscale photographs (halftones): always use a minimum of 300 dpi.
TIFF (or JJP): Bitmapped line drawings: use a minimum of 1000 dpi.
TIFF (or JJP): Combinations bitmapped line/half-tone (color or grayscale): a minimum of 500 dpi is required.

Please do not:
• Supply files that are optimized for screen use (e.g., GIF, BMP, PICT, WPG); the resolution is too low.
• Supply files that are too low in resolution.
• Submit graphics that are disproportionately large for the content.
Color artwork
Please make sure that artwork files are in an acceptable format (TIFF (or JPEG), EPS (or PDF), or MS Office files) and with the correct resolution. If, together with your accepted article, you submit usable color figures then Elsevier will ensure, at no additional charge, that these figures will appear in color online (e.g., ScienceDirect and other sites) regardless of whether or not these illustrations are reproduced in color in the printed version. **For color reproduction in print, you will receive information regarding the costs from Elsevier after receipt of your accepted article.** Please indicate your preference for color: in print or online only. **Further information on the preparation of electronic artwork.**

Figure captions
Ensure that each illustration has a caption. A caption should comprise a brief title (**not** on the figure itself) and a description of the illustration. Keep text in the illustrations themselves to a minimum but explain all symbols and abbreviations used.

Text graphics
Text graphics may be embedded in the text at the appropriate position. If you are working with LaTeX and have such features embedded in the text, these can be left. See further under Electronic artwork.

References

Citation in text
Please ensure that every reference cited in the text is also present in the reference list (and vice versa). Any references cited in the abstract must be given in full. Unpublished results and personal communications are not recommended in the reference list, but may be mentioned in the text. If these references are included in the reference list they should follow the standard reference style of the journal and should include a substitution of the publication date with either ‘Unpublished results’ or ‘Personal communication’. Citation of a reference as ‘in press' implies that the item has been accepted for publication.

Reference links
Increased discoverability of research and high quality peer review are ensured by online links to the sources cited. In order to allow us to create links to abstracting and indexing services, such as Scopus, CrossRef and PubMed, please ensure that data provided in the references are correct. Please note that incorrect surnames, journal/book titles, publication year and pagination may prevent link creation. When copying references, please be careful as they may already contain errors. Use of the DOI is highly encouraged.

A DOI is guaranteed never to change, so you can use it as a permanent link to any electronic article. An example of a citation using DOI for an article not yet in an issue is: VanDecar J.C., Russo R.M., James D.E., Ambeh W.B., Franke M. (2003). Aseismic continuation of the Lesser Antilles slab beneath northeastern Venezuela. Journal of Geophysical Research, https://doi.org/10.1029/2001JB000884. Please note the format of such citations should be in the same style as all other references in the paper.

Web references
As a minimum, the full URL should be given and the date when the reference was last accessed. Any further information, if known (DOI, author names, dates, reference to a source publication, etc.), should also be given. Web references can be listed separately (e.g., after the reference list) under a different heading if desired, or can be included in the reference list.

Data references
This journal encourages you to cite underlying or relevant datasets in your manuscript by citing them in your text and including a data reference in your Reference List. Data references should include the following elements: author name(s), dataset title, data repository, version (where available), year, and global persistent identifier. Add [dataset] immediately before the reference so we can properly identify it as a data reference. The [dataset] identifier will not appear in your published article.

References in a special issue
Please ensure that the words 'this issue' are added to any references in the list (and any citations in the text) to other articles in the same Special Issue.

Reference management software
Most Elsevier journals have their reference template available in many of the most popular reference management software products. These include all products that support **Citation Style Language styles**, such as Mendeley. Using citation plug-ins from these products, authors only need to select
the appropriate journal template when preparing their article, after which citations and bibliographies will be automatically formatted in the journal's style. If no template is yet available for this journal, please follow the format of the sample references and citations as shown in this Guide. If you use reference management software, please ensure that you remove all field codes before submitting the electronic manuscript. More information on how to remove field codes from different reference management software.

Users of Mendeley Desktop can easily install the reference style for this journal by clicking the following link:
http://open.mendeley.com/use-citation-style/the-journal-of-chemical-thermodynamics
When preparing your manuscript, you will then be able to select this style using the Mendeley plug-ins for Microsoft Word or LibreOffice.

Reference formatting

There are no strict requirements on reference formatting at submission. References can be in any style or format as long as the style is consistent. Where applicable, author(s) name(s), journal title/book title, chapter title/article title, year of publication, volume number/book chapter and the article number or pagination must be present. Use of DOI is highly encouraged. The reference style used by the journal will be applied to the accepted article by Elsevier at the proof stage. Note that missing data will be highlighted at proof stage for the author to correct. If you do wish to format the references yourself they should be arranged according to the following examples:

Reference style

Text: Indicate references by number(s) in square brackets in line with the text. The actual authors can be referred to, but the reference number(s) must always be given.
Example: '..... as demonstrated [3,6]. Barnaby and Jones [8] obtained a different result ....'

List: Number the references (numbers in square brackets) in the list in the order in which they appear in the text.
Examples:
Reference to a journal publication:
Reference to a journal publication with an article number:
Reference to a book:
Reference to a chapter in an edited book:
Reference to a website:
Reference to a dataset:

Journal abbreviations source

Journal names should be abbreviated according to the List of Title Word Abbreviations.

Video

Elsevier accepts video material and animation sequences to support and enhance your scientific research. Authors who have video or animation files that they wish to submit with their article are strongly encouraged to include links to these within the body of the article. This can be done in the same way as a figure or table by referring to the video or animation content and noting in the body text where it should be placed. All submitted files should be properly labeled so that they directly relate to the video file's content. In order to ensure that your video or animation material is directly usable, please provide the file in one of our recommended file formats with a preferred maximum size of 150 MB per file, 1 GB in total. Video and animation files supplied will be published online in the electronic version of your article in Elsevier Web products, including ScienceDirect. Please supply 'still' with your files: you can choose any frame from the video or animation or make a separate image. These will be used instead of standard icons and will personalize the link to your video data. For
more detailed instructions please visit our video instruction pages. Note: since video and animation cannot be embedded in the print version of the journal, please provide text for both the electronic and the print version for the portions of the article that refer to this content.

**Data visualization**

Include interactive data visualizations in your publication and let your readers interact and engage more closely with your research. Follow the instructions here to find out about available data visualization options and how to include them with your article.

**Supplementary material**

Supplementary material such as applications, images and sound clips, can be published with your article to enhance it. Submitted supplementary items are published exactly as they are received (Excel or PowerPoint files will appear as such online). Please submit your material together with the article and supply a concise, descriptive caption for each supplementary file. If you wish to make changes to supplementary material during any stage of the process, please make sure to provide an updated file. Do not annotate any corrections on a previous version. Please switch off the 'Track Changes' option in Microsoft Office files as these will appear in the published version.

**Research data**

This journal encourages and enables you to share data that supports your research publication where appropriate, and enables you to interlink the data with your published articles. Research data refers to the results of observations or experimentation that validate research findings. To facilitate reproducibility and data reuse, this journal also encourages you to share your software, code, models, algorithms, protocols, methods and other useful materials related to the project.

Below are a number of ways in which you can associate data with your article or make a statement about the availability of your data when submitting your manuscript. If you are sharing data in one of these ways, you are encouraged to cite the data in your manuscript and reference list. Please refer to the "References" section for more information about data citation. For more information on depositing, sharing and using research data and other relevant research materials, visit the research data page.

**Data linking**

If you have made your research data available in a data repository, you can link your article directly to the dataset. Elsevier collaborates with a number of repositories to link articles on ScienceDirect with relevant repositories, giving readers access to underlying data that gives them a better understanding of the research described.

There are different ways to link your datasets to your article. When available, you can directly link your dataset to your article by providing the relevant information in the submission system. For more information, visit the database linking page.

For supported data repositories a repository banner will automatically appear next to your published article on ScienceDirect.

In addition, you can link to relevant data or entities through identifiers within the text of your manuscript, using the following format: Database: xxxx (e.g., TAIR: AT1G01020; CCDC: 734053; PDB: 1XFN).

**Mendeley Data**

This journal supports Mendeley Data, enabling you to deposit any research data (including raw and processed data, video, code, software, algorithms, protocols, and methods) associated with your manuscript in a free-to-use, open access repository. During the submission process, after uploading your manuscript, you will have the opportunity to upload your relevant datasets directly to Mendeley Data. The datasets will be listed and directly accessible to readers next to your published article online.

For more information, visit the Mendeley Data for journals page.

**Data in Brief**

You have the option of converting any or all parts of your supplementary or additional raw data into one or multiple data articles, a new kind of article that houses and describes your data. Data articles ensure that your data is actively reviewed, curated, formatted, indexed, given a DOI and publicly available to all upon publication. You are encouraged to submit your article for Data in Brief as an additional item directly alongside the revised version of your manuscript. If your research article is
accepted, your data article will automatically be transferred over to *Data in Brief* where it will be editorially reviewed and published in the open access data journal, *Data in Brief*. Please note an open access fee of 600 USD is payable for publication in *Data in Brief*. Full details can be found on the *Data in Brief* website. Please use this template to write your Data in Brief.

**MethodsX**

You have the option of converting relevant protocols and methods into one or multiple MethodsX articles, a new kind of article that describes the details of customized research methods. Many researchers spend a significant amount of time on developing methods to fit their specific needs or setting, but often without getting credit for this part of their work. MethodsX, an open access journal, now publishes this information in order to make it searchable, peer reviewed, citable and reproducible. Authors are encouraged to submit their MethodsX article as an additional item directly alongside the revised version of their manuscript. If your research article is accepted, your methods article will automatically be transferred over to MethodsX where it will be editorially reviewed. Please note an open access fee is payable for publication in MethodsX. Full details can be found on the MethodsX website. Please use this template to prepare your MethodsX article.

**Data statement**

To foster transparency, we encourage you to state the availability of your data in your submission. This may be a requirement of your funding body or institution. If your data is unavailable to access or unsuitable to post, you will have the opportunity to indicate why during the submission process, for example by stating that the research data is confidential. The statement will appear with your published article on ScienceDirect. For more information, visit the **Data Statement page**.

**AFTER ACCEPTANCE**

**Online proof correction**

To ensure a fast publication process of the article, we kindly ask authors to provide us with their proof corrections within two days. Corresponding authors will receive an e-mail with a link to our online proofing system, allowing annotation and correction of proofs online. The environment is similar to MS Word: in addition to editing text, you can also comment on figures/tables and answer questions from the Copy Editor. Web-based proofing provides a faster and less error-prone process by allowing you to directly type your corrections, eliminating the potential introduction of errors. If preferred, you can still choose to annotate and upload your edits on the PDF version. All instructions for proofing will be given in the e-mail we send to authors, including alternative methods to the online version and PDF.

We will do everything possible to get your article published quickly and accurately. Please use this proof only for checking the typesetting, editing, completeness and correctness of the text, tables and figures. Significant changes to the article as accepted for publication will only be considered at this stage with permission from the Editor. It is important to ensure that all corrections are sent back to us in one communication. Please check carefully before replying, as inclusion of any subsequent corrections cannot be guaranteed. Proofreading is solely your responsibility.

**Offprints**

The corresponding author will, at no cost, receive a customized Share Link providing 50 days free access to the final published version of the article on ScienceDirect. The Share Link can be used for sharing the article via any communication channel, including email and social media. For an extra charge, paper offprints can be ordered via the offprint order form which is sent once the article is accepted for publication. Both corresponding and co-authors may order offprints at any time via Elsevier's Author Services. Corresponding authors who have published their article gold open access do not receive a Share Link as their final published version of the article is available open access on ScienceDirect and can be shared through the article DOI link.

**AUTHOR INQUIRIES**

Visit the Elsevier Support Center to find the answers you need. Here you will find everything from Frequently Asked Questions to ways to get in touch. You can also check the status of your submitted article or find out when your accepted article will be published.

© Copyright 2018 Elsevier | https://www.elsevier.com