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Manuscript Submission Requirements Checklist

- Articles published in *JCED* are distributed over five thematic sections. Authors are strongly encouraged to consult the specific guidelines that pertain to the five thematic section(s) appropriate for the scientific topic of their manuscript and, if applicable, also the guidelines for reporting data obtained from molecular modeling and simulation: Thermophysical and Thermochemical PropertiesVapor–Liquid Equilibria and Supercritical Fluid EquilibriaLiquid–Liquid Equilibria and Vapor–Liquid EquilibriaSolid–Solid Equilibria and Solid–Fluid EquilibriaAdsorption and Diffusion in Porous Materials
- If a manuscript is submitted that does not conform to the special requirements of *JCED*, it will be returned to the authors and not proceed to the Editor until the core requirements are met.
- Authors are strongly encouraged to utilize the 1-page <u>JCED Submission Checklist</u> to streamline both peer review and the NIST Statistical Editor's review.
- Upload the *JCED* Submission Checklist in ACS Paragon Plus as "Supporting Information for Review Only". By uploading this Checklist, the authors certify that they have read and followed the *JCED* Author Guidelines.
- In the experimental details, emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work.

Scope of the Journal

The Journal of Chemical & Engineering Data (JCED) is a monthly journal devoted to the publication of data on phase behavior and physical, thermodynamic, and transport properties obtained from **both** experiment and computation, which are viewed as complementary.

Examples of topics that are in-scope:

- Phase equilibrium or thermophysical/thermochemical properties of systems whose compositions are known. A reader must be able to make up the sample system in their laboratory and reproduce the data.
- New experimental phase equilibrium data (e.g., vapor-liquid, supercritical fluid, liquid-liquid, solid-solid, solid-liquid, solid-vapor, solid-supercritical fluid, and gas hydrate equilibrium).
- Thermophysical/thermochemical properties and phase equilibrium data obtained from quantum chemistry, molecular simulation, and molecular mechanics calculations
- Measurements of thermophysical properties (e.g., viscosities, speed of sound, ionic conductivities).
- Reviews of experimental techniques to measure phase equilibrium or thermophysical properties.

Examples of topics that are **NOT** in-scope:

- Phase equilibrium or thermophysical properties of mixtures whose compositions are **NOT** known. Many environmental and biological samples fit in this category.
- Reaction kinetics and catalysis.
- Applications that do not measure or calculate the fundamental thermophysical properties or

phase equilibria (e.g., permeabilities through membranes without measurement and calculation of solubility and diffusivity).

• Materials synthesis and characterization where the phase equilibrium and/or thermophysical properties are not the main focus of the paper.

Manuscript Types

Articles

Most publications in JCED are regular Articles.

- Articles should present **a significant amount** of experimental or computational data on properties of systems of technological or theoretical interest that are not available in the original literature, that have lower uncertainty than those published, or that help resolve conflicts in previously published values.
- Results must be discussed in detail and comparisons given to previously published results for the same or similar systems. Please use a database like *Thermolit* (<u>http://trc.nist.gov/thermolit/</u>) for comparison purposes.
- All articles must include substantive results and discussion of those results. *JCED* has special requirements on materials, uncertainties and presentation of results in tabular form. Please review the Data Table Requirements at <u>http://trc.nist.gov/JCED-Support.html</u>.

Reviews

Reviews on specific topics within the scope of *JCED*—thermophysical properties and phase equilibria from experiment and computation—are strongly encouraged.

- Reviews should be no longer than 8,000 words.
- While reviews are typically invited, pre-publication inquiries for reviews are welcome and should be sent to the Editor-in-Chief (<u>eic@jced.acs.org</u>).

Perspectives

Perspectives are interpretive accounts on subjects of current interest to the thermophysical properties research community. These articles reflect the opinions of the authors and are intended to be thought provoking. Perspectives should be at least 1500 words in length and include at least 30 references (avoiding an undue fraction of self-citations). Authors should be subject matter experts. It is recommended that authors obtain pre-approval from the Editor-in-Chief (eic@jced.acs.org) prior to unsolicited submission. Manuscripts submitted as Perspectives will undergo the usual peer review process.

Comments

Comments include significant remarks on work previously published in *JCED* and are restricted to two printed pages including tables, figures, text, and a brief abstract. If a Comment is concerned with the work of other authors, the Editor will permit those authors to reply. Comments should be used only when an important point is to be made. The Editor reserves the right to reject comments that are not substantive.

ACS Researcher Resources

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit <u>ACS</u> <u>Researcher Resources</u> for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- <u>Mastering the Art of Scientific Publication</u>, which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on <u>how to prepare and submit a manuscript</u> to the ACS Publications manuscript submission and peer review system, including details on selecting the applicable <u>Journal</u> <u>Publishing Agreement</u>.
- <u>Sharing your research</u> with the public through the ACS Publications open access program.
- <u>ACS Reviewer Lab</u>, a free online course covering best practices for peer review and related ethical considerations.
- <u>ACS Author Lab</u>, a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- <u>ACS Inclusivity Style Guide</u>, a guide that helps researchers communicate in ways that recognize and respect diversity in all its forms.

Manuscript Preparation

Submit with Fast Format

All ACS journals and partner journals have simplified their formatting requirements in favor of a streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers <u>here</u>.

Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- When required by a journal's structure or length limitations, manuscript templates should be used.
- References can be provided in any style, but they must be complete, including titles. For information about the required components of different reference types, please refer to the <u>ACS Style Quick Guide</u>.
- Supporting Information must be submitted as a separate file(s).

Document Templates and Format

The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates <u>here</u>.

General information on the preparation of manuscripts may also be found in the <u>ACS Guide to</u> <u>Scholarly Communication</u>.

Acceptable Software, File Designations, and TeX/LaTeX

See the list of <u>Acceptable Software</u> and appropriate <u>File Designations</u> to be sure your file types are compatible with the submission system. Information for manuscripts generated from <u>TeX/LaTeX</u> is also available.

Cover Letter

A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

The JCED cover letter must include:

- The manuscript title
- A statement of why the paper is appropriate for *JCED* and how it fits into *JCED*'s scope.
- The name and complete contact information (mailing address, telephone number, and e- mail address) of the corresponding author. The corresponding author must be a senior researcher, not a graduate student or post-doctoral researcher, and must have an ACS Paragon Plus ID (see section "Preparing for Submission" below).
- The names(s) of all coauthor(s). These will also need to be entered in ACS Paragon Plus in the same sequence as they appear on the first page of the manuscript. Upon submission, all authors are notified, so it is the corresponding author's responsibility to make sure that coauthors are listed and that all co-authors have approved the manuscript prior to submission. Deletion of an author after the manuscript has been submitted requires a confirmation letter addressed to the Editor-in-Chief from the author whose name is being deleted. For more information on ethical responsibilities of authors, see the <u>Ethical Guidelines to Publication of Chemical Research</u>.

Manuscript Text Components

The required components of every manuscript submission are described below.

Note that *Journal of Chemical & Engineering Data* has guidelines for each of five thematic sections and special requirements for Symbols, Units and Terminology, Reporting of Uncertainties, Nomenclature, Description of Chemical Samples and reporting of results in Tables.

- <u>Thermophysical and Thermochemical Properties</u>
- Vapor-Liquid Equilibria and Supercritical Fluid Equilibria
- Liquid–Liquid Equilibria and Vapor–Liquid–Liquid Equilibria
- Solid–Solid Equilibria and Solid–Fluid Equilibria
- Adsorption and Diffusion in Porous Materials

If applicable, authors may refer to the guidelines for reporting data obtained from <u>Molecular</u> <u>Modeling and Simulation</u>.

Table of Contents Graphic

A Table of Contents (TOC) graphic is required for all manuscripts upon submission. This graphic will also be used for the graphical abstract both in the published article and on the ACS website. The TOC graphic should capture reader attention and, in conjunction with the manuscript title, give readers quick visual context of the essence of the manuscript.

• The TOC graphic should be a distinct graphic, not identical to one of the figures from the

article.

- The TOC graphic should be 4 cm high and 8 cm wide. Larger images will be reduced to fit within those dimensions.
- Type size of labels, formulas, or numbers within the graphic must be legible.
- The graphic should be labeled "Table of Contents graphic".
- Tables or spectra are NOT acceptable in the TOC graphic.

Title

Use a specific rather than a general title. The title should be as brief and informative as possible.

Authorship

Provide given names (where some of the given names may be abbreviated as initials) and last name of each author and provide the e-mail addresses of at least the corresponding author. The name(s) of the author(s) to whom inquiries about the paper should be addressed should be marked with an asterisk. Give the name and complete mailing address(es) of the institution(s) where the work was conducted. If the current address is different, include it in a footnote on the title page. It is the responsibility of the submitting author to ensure that the manuscript and any revisions have the full approval of all co-authors.

Abstract

The abstract will be used directly by <u>Chemical Abstracts</u>. It should have a maximum length of 200 words. The individual systems, properties, and range of conditions studied should be given.

Text

All manuscripts must contain the following sections: Introduction, Experimental and/or Computational Methods, Results and Discussion, and Conclusions. Provide essential information in a concise fashion and avoid unnecessary duplication in text, tables, and graphs.

Symbols, Units, and Terminology

SI units must be used throughout the manuscript, and authors must adhere to the IUPAC recommendations regarding symbols, units, and terminology. Details and examples can be found at <u>http://physics.nist.gov/cuu/</u>. For more information see *Quantities, Units and Symbols in Physical Chemistry*, 3rd ed., RSC Publishing: Cambridge, U.K., 2007, ISBN 0-85404-433-7 and Taylor, B. N. *Guide to the Use of the International System of Units (SI)*, NIST Special Publication 811, NIST: Gaithersburg, MD, 1995.

In the text, tables, and figures of your JCED manuscript:

- The relationship between the physical quantity, numerical value, and unit must follow the "calculus of quantities." This means that the physical quantity = numerical value × unit, so physical quantity/unit = numerical value. Symbols should be italicized and units given in roman font. Examples: In (p/kPa), T/K, $10^{10} \cdot D/m^2 \cdot s^1$.
- The center dot is the appropriate symbol for multiplication (times 'x' sign will be accepted).
- The format of T = (273.15 to 303.15) K is preferred instead of T = 273.15 303.15 K.
- Authors may use mole fraction or mass fraction to define the chemical purity of composition.

Molality (with units of mol·kg¹) should be used for concentration of solutions. Molarity (with units of mol·m³) is not an acceptable unit of concentration for *JCED*.

• Symbols should be defined where they are first used in the text, equations, figures, and tables. As a result, there should be no need for a Nomenclature List or List of Symbols.

Reporting Uncertainty in Results

The Journal is concerned with the reporting and interpretation of experimental and computational results. Such results are of little use unless they are accompanied by a meaningful statement of uncertainty.

- The uncertainty of each measured variable must be given and combined in quadrature to give the uncertainty in the derived properties, which must be stated at a defined confidence interval.
- A detailed description on how the estimated uncertainties are obtained must be provided in the Supporting Information.
- The number of significant digits must not exceed one more digit than specified by the estimated uncertainty.
- The uncertainties of all reported quantities must be included in the data tables. Example sample tables can be found at http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in all manuscripts should closely match http://trc.nist.gov/JCED-Support.html and tables in the data are entered by NIST into their database, as part of our collaboration with the NIST Thermodynamics Research Center, so the data must be supplied in this fashion.

Help with how to determine uncertainties can be found in the *Guide to the Expression of Uncertainty in Measurement*, ISO, October, 1993. The recommendations in this publication have been succinctly presented in Chirico et al. *J. Chem. Eng. Data* **2003**, *48*, 1344–1359 and *Guidelines for the Evaluation and Expression of Uncertainty in NIST Measurement Results*, NIST Technical Note 1297; Taylor, B. N.; Kuyatt, C. E.; NIST: 1994 which can be found at the following website <u>http://physics.nist.gov/cuu/</u>.

Chemical Nomenclature and Sample Purity

- The IUPAC systematic names for the chemical substances studied must be provided. Assistance with the IUPAC nomenclature can be found at <u>http://www.chem.qmul.ac.uk/iupac/</u>. Authors must also provide either the CAS registry number or a 2D chemical structure.
- Once the IUPAC systematic name has been provided, it is acceptable for authors to define either a common name or acronym and for this to be used for the remainder of the text, tables, and figures.
- The origin, purification method, purity, and method of purity determination of all chemicals used must be included and put in a table. The table should look exactly like the one found at <u>http://trc.nist.gov/JCED-Support.html</u>. This information is necessary for our partnership with the NIST Thermodynamics Research Center, so the information must be supplied in this fashion.
- For non-commercial synthesized substances, their preparation and analytical methods used for determination the chemical compositions should specified. For chemical substances obtained from commercial suppliers, the purities must be determined (e.g., using gas chromatography). Where applicable, the purification method needs to be included.
- If ¹H-nuclear magnetic resonance (NMR) data are used to quantify the purity of a chemical sample, authors must provide a copy of the NMR spectrum, including chemical shifts and experimental peak integrals in the Supporting Information. NMR Guidelines can be found at

Tables

Properly formatted Tables are critical to our collaboration with the TRC at NIST. Tables must be exactly as shown in the examples at <u>http://trc.nist.gov/JCED-Support.html</u>.

- Tables should be numbered with Arabic numbers.
- The table title should appear immediately above the table (not below) and should indicate the contents of the table; the title should contain definitions of all symbols in the table and be sufficiently comprehensive to stand alone, independent of the text.
- The symbols for physical quantities used in the headings of columns or rows must be defined in the table footnotes.
- The measured values or the averages of several measured values should be given.
- Tables of smoothed or derived values will NOT be published except in circumstances where the values are difficult to represent by an equation and the raw values are difficult to use (e.g., parameters for fits to Langmuir adsorption isotherm, thermal functions calculated from heat capacity measurements).
- Uncertainties for all reported quantities must be provided either in the body of the table or as footnotes.

Figures

- Figures showing the trends of the data must be accompanied by Tables of the actual experimental values.
- Deviations of the measured values from either a smoothing equation or other correlations from the literature are preferred.
- Plots must include values of the phase behavior or physical property published by other workers when available.
- Symbols and lines must be defined in the figure caption. Figure axis labels must obey the calculus of quantities and use symbols, not words, for physical quantities.
- Examples of acceptably formatted figures for various data types are available at https://trc.nist.gov/JCED-Support.html.
- Illustrations and their captions may be embedded in the text (preferred) or inserted at the end of the manuscript.
- We encourage the use of color in figures to enhance the understanding of the science being displayed. Please use symbols both of different color and different shapes. Note that the color of symbols appearing in color figures cannot be reproduced within the figure captions.

Equations

Equations should be numbered consecutively, and subscripts and superscripts should be evident. When a correlating equation is used to fit results, the units of the variables should be contained within the equation and the numerical values of the parameters should be given in a table of the coefficients for the equation. Designate equations by, for example, eq 1 or eqs 1 to 3.

Safety

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with

the reported work. This information should be in the experimental details section of the full article or communication.

Acknowledgments

Include only necessary credits in the Acknowledgment section at the end of the text.

Additional Information

Additional information that is not essential to the main body of the manuscript should be placed in a separate **Supporting Information** file and uploaded as "Supporting Information for Publication" in ACS Paragon Plus.

- The Supporting Information file must begin with the manuscript title and authorship as it appears at the beginning of the main manuscript.
- The main manuscript should include tables showing all of the reported quantities with their uncertainties. However, exceptions can be made when there is an excessively large amount of reported data. In such cases, the tables of data and uncertainties can be placed in the Supporting Information.
- Other information that might be appropriate as Supporting Information would include long derivations, spectra, and analytical results regarding sample purity.

Supporting Information

This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of <u>Acceptable Software by File</u> <u>Designation</u> and confirm that your Supporting Information is <u>viewable</u>.

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief, nonsentence description of the actual contents of each file, including the file type extension, is required. This description should be labeled Supporting Information and should appear before the Acknowledgement and Reference sections. Examples of sufficient and insufficient descriptions are as follows:

Examples of sufficient descriptions: "Supporting Information: ¹H NMR spectra for all compounds (PDF)" or "Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)".

Examples of insufficient descriptions: "Supporting Information: Figures S1-S3" or "Additional figures as mentioned in the text".

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

Research Data Policy

All ACS journals strongly encourage authors to make the research data underlying their articles publicly available at the time of publication.

Research data is defined as materials and information used in the experiments that enable the validation of the conclusions drawn in the article, including primary data produced by the authors for the study being reported, secondary data reused or analyzed by the authors for the study, and any other materials necessary to reproduce or replicate the results.

The <u>ACS Research Data Policy</u> provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

If a submitted manuscript does not conform to the special requirements of *JCED*, it will be returned to the authors and not considered for peer review until the Checklist is completed and Author Guidelines are followed. Authors are strongly encouraged to complete and submit the <u>JCED</u> <u>Submission Checklist</u>, which outlines the journal's data requirements.

Language and Editing Services

A well-written paper helps share your results most clearly. ACS Publications' <u>English Editing</u> <u>Service</u> is designed to help scientists communicate their research effectively. Our subject-matter expert editors will edit your manuscript for grammar, spelling, and other language errors so your ideas are presented at their best.

Preparing Graphics

The quality of illustrations in ACS journals and partner journals depends on the quality of the original files provided by the authors. Figures are not modified or enhanced by journal production staff. All graphics must be prepared and submitted in digital format.

Graphics should be inserted into the main body whenever possible. Please see Appendix 2 for additional information.

Any graphic (figure chart, scheme, or equation) that has appeared in an earlier publication should include a <u>credit line</u> citing the original source. Authors are responsible for <u>obtaining written</u> <u>permission</u> to re-use this material.

Figure and Illustration Services

The impact of your research is not limited to what you can express with words. Tables and figures such as graphs, photographs, illustrations, diagrams, and other visuals can play a significant role in effectively communicating your findings. Our <u>Artwork Editing</u> and <u>Graphical Abstract</u> services generate publication-ready figures and Table of Contents (TOC) graphics that conform to your chosen journal's specifications. For figures, this includes changes to file type, resolution, color space, font, scale, line weights, and layout (to improve readability and professional appearance). For TOC graphics, our illustrators can work with a rough sketch or concept or help extract the key findings of your manuscript directly for use as a visual summary of your paper.

Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through <u>ACS Publishing Center</u>, which requires an

ACS ID to log in. Registering for an ACS ID is fast, free, and does not require an ACS membership. Please refer to Appendix 1 for additional information on preparing your submission

Prior Publication Policy

<u>Journal of Chemical & Engineering Data</u> authors are allowed to deposit an initial draft of their manuscript in a preprint service such as <u>ChemRxiv</u>, bioRxiv, and arXiv prior to submission to the journal. Please note any use of a preprint server in the cover letter and include a link to the preprint, and as appropriate, state how the manuscript has been adjusted/updated between deposition and submission. All other prior/redundant publication is forbidden.

Upon publication in *Journal of Chemical & Engineering Data*, authors are advised to add a link from the preprint to the published paper via the Digital Object Identifier (DOI). Some services, such as ChemRxiv and bioRxiv, add this link for authors automatically after publication.

Providing Potential Reviewer Names

Suggest **at least 4** possible reviewers. Ideally, suggested referees will work in different countries from the authors. Authors are encouraged to avoid suggesting reviewers from the authors' institutions. Do not suggest reviewers who may have a <u>real or perceived conflict of interest</u>. Whenever possible, suggest academic email addresses rather than personal email addresses.

Manuscript Transfer

If your submission is declined for publication by this journal, the editors might deem your work to be better suited for another ACS Publications journal or partner journal and suggest that the authors consider transferring the submission. <u>Manuscript Transfer</u> simplifies and shortens the process of submitting to another ACS journal or partner journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied to the new draft submission. Authors are free to accept or decline the transfer offer.

Note that each journal is editorially independent. Transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor of the next journal.

PRODUCTION AND PUBLICATION

Proofs via ACS Direct Correct

Correction of the galley proofs is the responsibility of the Corresponding Author. The Corresponding Author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via <u>ACS Direct Correct</u>. Extensive or important changes on page proofs, including changes to the title or list of authors, are subject to review by the editor.

It is the responsibility of the Corresponding Author to ensure that all authors listed on the manuscript agree with the changes made on the proofs. Galley proofs should be returned within 48 hours in order to ensure timely publication of the manuscript.

Publication Date and Patent Dates

Accepted manuscripts will be published on the ACS Publications Web site as soon as page proofs are corrected and all author concerns are resolved. The first date on which the document is published on the Web is considered the publication date.

Publication of manuscripts on the Web may occur weeks in advance of the cover date of the issue of publication. Authors should take this into account when planning their patent and intellectual property activities related to a document and should ensure that all patent information is available at the time of first publication, whether ASAP or issue publication.

All articles published ahead of print receive a unique Digital Object Identifier (DOI) number, which is used to cite the manuscript before and after the paper appears in an issue. Additionally, any supplemental information submitted along with the manuscript will automatically be assigned a DOI and hosted on Figshare to promote open data discoverability and use of your research outputs.

ASAP Publication

Manuscripts will be published on the "ASAP Articles" page on the web as soon as page proofs are corrected and all author concerns are resolved. ASAP publication usually occurs within a few working days of receipt of page proof corrections, which can be several weeks in advance of the cover date of the issue.

Post-Publication Policies

The American Chemical Society follows guidance from the <u>Committee on Publication Ethics</u> (COPE) when considering any ethical concerns regarding a published article, Retractions, and Expressions of Concern.

Additions and Corrections

Additions and Corrections may be requested by the author(s) or initiated by the Editor to address important issues or correct errors and omissions of consequence that arise after publication of an article. All Additions and Corrections are subject to approval by the Editor, and should bring new and directly relevant information and corrections that fix scientific facts. Minor corrections and additions will not be published. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work.

Additions and Corrections must be submitted as new manuscripts via the ACS Publishing Center by the Corresponding Author for publication in the "Addition/Correction" section of the Journal. The corresponding author should obtain approval from all coauthors prior to submitting or provide evidence that such approval has been solicited. The manuscript should include the original article title and author list, citation including DOI, and details of the correction.

Retractions

Articles may be retracted for scientific or ethical reasons and may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. Articles that contain seriously flawed or erroneous data such that their findings and conclusions

cannot be relied upon may be retracted in order to correct the scientific record. When an article is retracted, a notice of Retraction will be published containing information about the reason for the Retraction. The originally published article will remain online except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks).

Expressions of Concern

Expressions of Concern may be issued at the discretion of the Editor if:

- there is inconclusive evidence of research or publication misconduct by the authors;
- there is evidence that the findings are unreliable but the authors' institution will not investigate the case;
- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
- an investigation is underway but a judgment will not be available for a considerable time.

Upon completion of any related investigation, and when a final determination is made about the outcome of the article, the Expression of Concern may be replaced with a Retraction notice or Correction.

Sharing Your Published Article

At ACS Publications, we know it is important for you to be able to share your peer reviewed, published work with colleagues in the global community of scientists. As sharing on sites known as scholarly collaboration networks (SCNs) is becoming increasingly prevalent in today's scholarly research ecosystem, we would like to remind you of the many ways in which you, a valued ACS author, can <u>share your published work</u>.

Publishing open access makes it easy to share your work with friends, colleagues, and family members. In addition, ACS Publications makes it easy to share your newly published research with ACS Articles on Request (see below). Don't forget to promote your research and related data on social media, at conferences, and through scholarly communication networks. Increase the impact of your research using the following resources: <u>Altmetrics</u>, <u>Figshare</u>, <u>ACS Certified Deposit</u>

E-Prints

When your article is published in an ACS journal or partner journal, corresponding authors are provided with a link that offers up to 50 free digital prints of the final published work. This link is valid for the first 12 months following online publication, and can be shared via email or an author's website. After one year, the access restrictions to your article will be lifted, and you can share the <u>Articles on Request</u> URL on social media and other channels. To access all your Articles on Request links, log in to your ACS Researcher Resources account and visit the "My Published Manuscripts" page.

Reprints

Article, journal, and commercial reprints are available to order.

Appendix 1: PREPARING FOR SUBMISSION

We've developed ACS' publishing and editorial policies in consultation with the research communities that we serve, including authors and librarians. Browse our policies below to learn more.

Ethical Guidelines

ACS editors have provided <u>Ethical Guidelines</u> for persons engaged in the publication of chemical research—specifically, for editors, authors, and reviewers. Each journal also has a specific <u>policy</u> <u>on prior publication</u>.

OFAC Compliance

As a U.S.-based non-profit organization, the American Chemical Society (ACS) is required to comply with U.S. sanctions laws and regulations administered by the <u>U.S. Treasury Department's</u> <u>Office of Foreign Assets Control (OFAC)</u>. While these laws and regulations permit U.S.-based publishers like ACS to engage in publishing-related activities with authors located in sanctioned regions in many cases, ACS may be prohibited under U.S. law from engaging in publishing-related activities in some cases, including, but not limited to, instances where an author or the institution with which an author is affiliated is located in a particular sanctioned region or has been designated by OFAC as a <u>Specially Designated National</u> (SDN) pursuant to certain U.S. sanctions programs. ACS reserves the right to refrain from engaging in any publishing-related activities that ACS determines in its sole discretion may be in violation of U.S. law.

Safety Considerations

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the <u>Safety Statement</u> <u>Style Sheet</u> and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* is freely available here.

Conflict of Interest Disclosure

A statement describing any financial conflicts of interest or lack thereof is published in each ACS journal and partner journal article.

During the submission process, the Corresponding Author must provide a statement on behalf of all authors of the manuscript, describing all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest. If the manuscript is accepted, the statement will be published in the final article.

If the manuscript is accepted and no conflict of interest has been declared, the following statement will be published in the final article: "The authors declare no competing financial interest."

Plagiarism

In publishing only original research, ACS is committed to deterring plagiarism, including selfplagiarism. ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process.

Further information about plagiarism can be found in Part B of the <u>Ethical Guidelines to Publication</u> <u>of Chemical Research</u>. See also the <u>press release</u> regarding ACS' participation in the CrossCheck initiative.

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Appendix 2: Preparing Graphics

Resolution

Digital graphics pasted into manuscripts should have the following minimum resolutions:

- Black and white line art, 1200 dpi
- Grayscale art, 600 dpi
- Color art, 300 dpi

Size

Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (allow 12 pts. For each line of caption text). Lettering should be no smaller than 4.5 points in the final published format. The text should be legible when the graphic is viewed full-size. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

Color

Color may be used to enhance the clarity of complex structures, figures, spectra, and schemes, etc., and color reproduction of graphics is provided at no additional cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

Consult the Guidelines for <u>Table of Contents/Abstract Graphics</u> for specifications. Our team of subject-matter experts and graphical designers can also help generate a compelling TOC graphic to convey your key findings. Learn more about our <u>Graphical Abstract service</u>.

Figures

A caption giving the figure number and a brief description must be included below each figure. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

Charts

Charts (groups of structures that do not show reactions) may have a brief caption describing their contents.

Tables

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter-relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

Schemes

Each scheme (sequences of reactions) may have a brief caption describing its contents.

Chemical Structures

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

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