

Last updated: December 29, 2023 [View the latest guidelines online](#)

Scope of the Journal

[Organometallics](#) is the flagship journal of organometallic chemistry and records progress in one of the most active fields of science, bridging organic and inorganic chemistry. The journal publishes original content on fundamental experimental and theoretical/computational studies of all aspects of organometallic chemistry that depicts research on the synthesis, structure, bonding, chemical reactivity, and reaction mechanisms for a variety of applications, including catalyst design and catalytic processes; main-group, transition-metal, and lanthanide and actinide metal chemistry; synthetic aspects of polymer science, materials science, and solid-state chemistry; green chemistry; energy and environmental science; and bioorganometallic chemistry. Incremental contributions are not encouraged without justification.

For the purposes of this journal, an “organometallic” compound is defined as one in which there is a bonding interaction between one or more carbon atoms of an organic group or molecule and a main-group, transition, lanthanide, or actinide metal atom (or atoms). Following longstanding tradition, organic derivatives of the metalloids (such as boron, silicon, and the like) are included in this definition. Furthermore, manuscripts dealing with metal-containing compounds that do not have metal–carbon bonds will be considered if there is a close relationship between the subject matter and the principles and practice of organometallic chemistry. Such compounds may include, among other things, representatives from the following classes: molecular metal hydrides; metal alkoxides, thiolates, amides, and phosphides; metal complexes containing organo-group 15 and 16 ligands; metal nitrosyls. Manuscripts dealing with certain aspects of organophosphorus, organoselenium, and organosulfur chemistry also will be considered. In evaluating submissions that deal with subject matter that is peripheral to mainstream organometallic chemistry, the primary consideration is whether the manuscript is of interest to our readers.

If you are a new *Organometallics* author, or if you have not submitted a manuscript during the past year, please read and familiarize yourself with these complete Author Guidelines to ensure you are up to date with all of the journal’s manuscript preparation and submission requirements.

Editors, Authors, and Reviewers should read the [ACS Ethical Guidelines](#).

Manuscript Types

Articles (full papers) should be comprehensive and critical accounts of solutions to important problems. Articles based upon work reported in a preliminary communication or letter are welcome, *provided that they represent a substantial amplification and extension of the earlier work* and do not merely add experimental details or a few further examples. The earlier work must be prominently cited, mentioned in the cover letter, and uploaded for the convenience of reviewers and editors. For Articles, the bulk of the experimental section should be presented in the main text.

Communications are meant to provide rapid, preliminary publication of new developments in organometallic chemistry that will be of particular significance and interest to readers and promise to influence the future work and thinking of other chemists. Communications must convey the scientific findings concisely in abstract, main text, and graphical elements as determined by word count not exceeding 2,200 words, including titles/footnotes/captions of approximately five graphics

(the total height of all combined figures not to exceed 20 cm/8 inches in a single column); the TOC graphic is counted as one of the five graphics but is not counted against the total height. References are not included in word count to allow article titles to be included at submission. Authors no longer need to fit the manuscript to the strict pages by the template measure, but communications exceeding the word count limit must be shortened before acceptance. The standard communication length is a traditional four printed pages or less, however shorter “Flash Communications” of two traditional pages that report more focused results are encouraged.

Tutorials and Reviews are currently invitation only; suggestions for both authors and topics are welcome (chirik-office@orgmet.acs.org). **Tutorials** are meant to be resources for researchers, students, and instructors in advanced undergraduate and graduate courses. Formal requirements are minimal, and authors are free to present the topic with their own personal flavor and perspective. Additional media resources (slides, videos, etc.) are encouraged as Supporting Information; author photographs and biographical sketches are required (see Manuscript Text Components).

ACS Publishing Center

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 the [ACS Publishing Center](#) for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- [Mastering the Art of Scientific Publication](#), which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on [how to prepare and submit a manuscript](#) to ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, including details on selecting the applicable [Journal Publishing Agreement](#).
- [Sharing your research](#) with the public through the ACS Publications open access program.
- [ACS Reviewer Lab](#), a free online course covering best practices for peer review and related ethical considerations.
- [ACS Author Lab](#), a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- [ACS Inclusivity Style Guide](#), 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 [here](#).

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 [ACS Style Quick Guide](#).
 - 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 [here](#).

General information on the preparation of manuscripts may also be found in the [ACS Guide to Scholarly Communication](#).

Acceptable Software, File Designations, and TeX/LaTeX

See the list of [Acceptable Software](#) and appropriate [File Designations](#) to be sure your file types are compatible with ACS Paragon Plus. Information for manuscripts generated from [TeX/LaTeX](#) 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.

Authors must explain clearly and convincingly in their cover letter how their manuscript is original, significant, and novel and why it will be of interest to the readers of *Organometallics*. Authors should note if the manuscript has been previously declined by another journal, and along with the manuscript upload copies of all earlier correspondence and reviewer reports as an appendix to the cover letter, or as “supporting information for review only”. The authors must note in detail the revisions that have been made in response to previous reviewer reports and/or Editor input (color or bold/italics coding recommended).

Manuscript Text Components

The sections of an Article are:

- Title
- Authors' names and institutional addresses
- Graphic for Table of Contents and Abstract
- Abstract
- Introduction
- Results
- Discussion (may be combined with Results)
- Conclusion
- Experimental or Computational Section

- Associated Content (including Supporting Information statement)
- Author Information
- Acknowledgments
- References and Footnotes
- Supporting Information (including any CIF files, if not accommodated by CCDC, or computational files)

Communications will normally not have sections labeled Introduction, Results, Discussion, or Conclusions, although a limited number of subheadings may be justified in certain cases.

Tutorials and Reviews may follow the Article section format or include different or additional sections as necessary to present the material in a logical manner.

Claims of priority, originality, convenience, effectiveness, or value should be avoided or used with great restraint in the Title, Abstract, and throughout the manuscript. For example, the words “convenient,” “efficient,” “elegant,” “expedient,” “facile,” “first,” “new,” “novel,” “practical,” “simple,” “unique,” “unprecedented,” and “versatile” should not be used. In addition, editors may ask authors to moderate or remove what they judge to be excessive use of subjective evaluative language elsewhere in the manuscript.

Title. The title should be descriptive of the topic of the article and as short as possible, using easily searchable keywords and minimizing hyphenation. Avoid using abbreviations and acronyms unless they are more commonly used than spelled out words. Also avoid complex compound names as much as possible in the title by using generic names, and spell out elements rather than using symbols unless part of a compound name. Neither the title nor any other text should indicate that the paper is part of a numbered series on a broader research topic, or a numbered contribution from a particular institution or research group.

Abstract and Abstract/Table of Contents Graphic. The abstract should briefly state the purpose of the research, principal results, and major conclusions and not exceed 200 words. Undefined nonstandard abbreviations and reference citation numbers should be avoided. A graphic must be included with each manuscript for display in the Abstract and Table of Contents (TOC), fitting in an area no larger than 8.25 cm by 4.45 cm (3.25 inches by 1.75 inches). *The TOC graphic should not exactly duplicate a graphic appearing within the text of the manuscript.*

A well-written abstract together with the graphic and article Title and can attract the attention of potential readers and increase the likelihood that the published article will be cited by other researchers. In preparing an Abstract/TOC graphic, creativity is welcome, but avoid images of people living or from the past and avoid caricatures or parodies that could be socially/culturally insensitive or considered racist or discriminatory, especially when taken out of context. Ensure that cartoon depictions of machinery, nature, and processes do not indicate actions or settings that are improbable. See Appendix 2 for full details on graphics requirements.

Introduction. The introduction should include sufficient background information to provide appropriate context as to the novelty and importance of the new work and clearly state the purpose and objectives of the research. An extensive review of prior work is not appropriate, and documentation of the relevant background literature should be selective rather than exhaustive, particularly if reviews can be cited. Articles may use the heading “Introduction;” however, the opening paragraphs of some manuscript types may serve a similar function, although they are not labeled “Introduction.”

Results and Discussion Sections. The presentation of experimental details in the Results section should be kept to a minimum. Reiteration of information from tables, figures, or reaction schemes should be avoided. If the table, figure or reaction scheme refers to work or mechanistic proposals reported by others, add the relevant reference to the caption. For structures, line drawings are typically preferred over ball-and-stick representations. Separate Results and Discussion sections can be advantageous. The experimental or computational data in a Results section should normally be as valid 10 years from now as they are today. The analyses and models developed should then be provided in a Discussion section, keeping in mind that some of this information may be time-dependent, particularly as new data become available or instrumental or computational methods develop. Certain types of routine results of lesser interest to general readers (spectra of routine monitored reactions, tabular data generated from computer programs, chromatograms establishing (enantiomeric) purities, graphs, etc.) are often best presented in "Supporting Information for Publication."

Conclusion. A conclusions section is strongly recommended. If used, the content should not substantially duplicate the abstract or preceding text.

Experimental Section. Every manuscript reporting the results of experimental work must include an experimental section. This should describe all methods and procedures in sufficient detail to permit repetition of the work by others. It may precede or follow the Results and Discussion section(s). The past tense should be used throughout.

For Articles, the bulk of the experimental section should be presented in the main text. Supporting Information should only be used to describe the syntheses and characterization of derivative compounds: for example, the preparation of an isotopically labeled species by an otherwise known procedure or a salt with an alternative counteranion. Characterization data for known organic compounds prepared using a new catalyst would also be appropriate for Supporting Information.

For Communications, the experimental section should at a minimum document all data relevant to the "title compounds" or experiments and should be published as Supporting Information.

A "General Methods" paragraph may be provided to document protocols (such as purification methods and spectroscopic and chromatographic analyses) that are common to most of the individual procedures. It should be placed at the beginning of the experimental section. Alternatively, a reference to the General Methods paragraph in an earlier publication may be provided. Sources of reactants, reagents, and solvents need not be identified except for (1) starting compounds that are unusual or not widely available and (2) materials for which the author has evidence that the source is critical to the outcome of an experiment. Experiments involving a catalyst, enzyme, or reagent that is neither commercially available nor prepared by a described or clearly cited nonproprietary method may not be reported.

References. Authors should be judicious in citing the literature; unnecessarily long lists of references should be avoided. If a number of publications are relevant to a statement in the text, not more than two or three of the most seminal or recent should be cited; if appropriate, the author may add "and references cited therein" following a reference. Authors must also cite any previously published work wherein portions of the submitted work have been disclosed. It is seldom necessary or appropriate for an author to cite more than 10 of their own publications. No reference should repeat a reference that appears elsewhere in the manuscript's list of references. Long endnotes should be avoided; peripheral discussion should be placed in the Supporting Information. Endnotes should not contain graphics, experimental procedures, or compound

characterization data.

Author photographs and biographical sketches. For all Invited Reviews and Tutorials, a high-resolution (300 dpi or better), in focus, color head-and-shoulders photograph and a brief two or three sentence bio for each author should be included in the Author Information section.

Alternatively, a group photo of the authorship team may be used. Model release and copyright forms are required for author photographs and will be provided by the Journal office.

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 [Acceptable Software by File Designation](#) and confirm that your Supporting Information is [viewable](#).

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 [ACS Research Data Policy](#) provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

Nomenclature

It is the authors' responsibility to provide correct, informative, and unambiguous nomenclature that conforms to current usage (see *The ACS Style Guide* for guidance). Systematic names similar to

those employed by Chemical Abstracts Service (CAS) and the International Union of Pure and Applied Chemistry (IUPAC) are encouraged. However, rigid and consistent conformance to these recommendations is challenging with organometallic compounds. The nomenclature employed should at a minimum accurately give the stoichiometric and topological composition of a compound.

All compounds should be referred to by the same name, abbreviation, number, or symbol throughout the text and graphics. For example, a manuscript that randomly mixes the expressions “PPh₃”, “P(C₆H₅)₃”, “Ph₃P”, and “triphenylphosphine” is not acceptable. In rare instances, a case can be made that two representations of the same compound are required.

Abbreviations

A list of accepted abbreviations may be found in Appendix 10-2 of *The ACS Style Guide*. Appropriate formats for units are summarized in Chapter 11. Symbols for physical quantities should be italicized (for example, *c*, *E_a*, *J*, *m/z*, *t_{1/2}*).

Experimental Section: Syntheses

Each paragraph describing a synthesis experiment should begin with the name of the product and any structure number assigned to the compound in the Results section. Thereafter, the compound should be identified by its structure number. Use of standard abbreviations or unambiguous molecular formulas for reagents and solvents, and of structure numbers rather than chemical names to identify starting materials and intermediates, is encouraged.

Reactant and product quantities should be given in both weight and molar units. It should be unambiguous whether yields pertain to a crude product (specify purity if possible) or a purified product. If yields are determined chromatographically, details (standards, response factors, means of correlating the peak to a structure, etc.) should be provided. The Editors would like to point out that reported yields above 95%, isomer ratios above 200:1, and enantiomeric excesses above 99% typically aren't realistic without further explanation.

The Editors encourage authors to emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work, including the use of toxic and/or environmentally persistent reagents and solvents, and provide a rationale on choice of these reagents and solvents. *Organometallics* further encourages authors to consider the Principles of Green Chemistry in carrying out their research and consider reporting metrics such as atom economy, mass efficiency, E-factor, or others. For more information, please consult [Research Tools](#) provided by the ACS Green Chemistry Institute.

Authors are responsible for retaining their original data or having available original data from collaborators or from contractors who perform analyses on their behalf. Authors may be asked to provide copies of spectra or analytical reports if an editor or reviewer raises a question about reported results.

Experimental Section: Compound Characterization

The Journal upholds a high standard for compound characterization to ensure that substances being added to the chemical literature have been correctly identified and can be synthesized in known yield and purity by the reported preparation and isolation methods. The editors remind

authors that it is unethical to modify reported data or spectra, for example to correct spectral baselines or remove solvent or impurity peaks.

For all **new** compounds, evidence adequate to establish both *identity* and *degree of purity* (homogeneity) must be provided.

For known compounds prepared by a new or modified synthetic procedure, the types of physical and spectroscopic data that were found to match *cited* literature data should be identified, and purity documentation should be provided.

Purity. For all new compounds, *Organometallics* requires a clear statement in the Experimental Section explaining how purity has been established. This may be included under General Considerations, or in the paragraphs providing synthetic details.

Organometallics strongly encourages the characterization of all new compounds by elemental analysis. For such data, agreement of calculated and found values within 0.4% (e.g., Calcd: 20.14%; Found: 20.54%) is considered acceptable. For deviations slightly outside the accepted range, authors are encouraged to provide an explanation in the relevant paragraph of the Experimental section, and to include a statement such "although these results are outside the range viewed as establishing analytical purity, they are provided to illustrate the best values obtained to date."

Where satisfactory combustion analysis data cannot be obtained, alternative characterization data must be provided as evidence of bulk purity, e.g. clean NMR spectra in the Supporting Information (^1H and ^{13}C required for diamagnetic compounds; ^{31}P and other nuclei encouraged when relevant). These NMR data should be formatted per the [NMR Guidelines for ACS Journals](#).

If the bulk purity of a compound cannot be established, the authors should clearly disclose and justify this in the paper.

If the isolation of a pure compound is not being claimed, the degree of purity must still be estimated and (for diamagnetic compounds) NMR data supplied as described above. Peaks not belonging to the compound should be designated and assigned where possible.

High-resolution mass spectroscopic data, including "exact mass" determinations of molecular ions, do not address the purity of the product (they do support the identity of the product).

Identity.

NMR Spectroscopy. For all new diamagnetic substances, NMR data should be reported (^1H , ^{13}C , and relevant heteronuclei). This should include the field strength, the solvent, any nuclei being decoupled, and other parameters as detailed in the [NMR Guidelines for ACS Journals](#). Spectra of new compounds must be depicted in the Supporting Information, formatted as described in the NMR Guidelines. Any 2D methods used to aid in peak assignments should be described. It is strongly recommended that NMR signals be assigned and coupling constants be labeled as $^nJ_{\text{HX}}$ when relevant.

Primary NMR Data Files. Submission of primary NMR data files (FID files, acquisition data, processing parameters) is highly recommended. All original primary NMR data supporting a

submission should be retained and provided if requested. For more information on packaging primary NMR data and metadata for submission, see the [ACS Research Data Center](#).

When submitting FID files:

- One folder should be created for each compound
- Folder should be named clearly, using the compound number
- Include the FID files, acquisition data and processing parameters for each experiment
- Name each spectrum according to the type of nucleus measured: ^1H , ^{13}C , DEPT, COSY, etc.
- NMR files should be compressed into zip file(s)

In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e., 300 MHz ^1H or 50 MHz ^{13}C). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

Optical Spectroscopy. It is strongly recommended that, when feasible, new substances be characterized by IR spectroscopy. It is sufficient to report the most diagnostic or intense absorptions. Similarly, it is recommended that colored substances be characterized by UV/visible spectroscopy, particularly when the spectrum is more complex than a featureless tail into the visible region.

Crystallographic Data. Single-crystal X-ray diffraction results are not acceptable as the only means of characterization of new compounds.

Crystal Structure Quality Standards. Crystal structure determinations reported in Organometallics should adhere to commonly accepted standards of rigor and presentation. Accordingly, only carefully collected and satisfactorily refined structures should be considered for inclusion in a manuscript.

Note that CIFs, structure factor tables, and checkCIF reports for organic, metal-organic, and inorganic structures must be submitted to the Cambridge Crystallographic Data Centre (CCDC) prior to manuscript submission. The CCDC deposition number(s) should be entered into ACS Paragon Plus during submission. In addition, authors are required to upload the checkCIF output files (combined into one PDF file) as Supporting Information for Review Only. Any A and/or B level alerts must also be addressed prior to submission or otherwise explained in the checkCIF PDF. See [Requirements for Depositing X-Ray Crystallographic Data](#) for complete details on submission of CIFs. Any subsequent revisions to the CIFs or structure factor tables should be deposited directly with the CCDC before uploading a revised manuscript to ACS Paragon Plus.

Reviewers will have access via the CCDC to an electronic copy of the CIF(s) associated with a manuscript. For many reviewers, an electronic CIF greatly simplifies the review process. Thus, the lack of availability of an electronic CIF may result in significant delays in the review process. If the manuscript is accepted and published, the CIF(s) will be made available to readers via the ACS Publications Web site.

CCDC will accept organic, metal-organic, and inorganic compounds, including extended molecular solids and powder data where a constrained refinement has been used. Structural data for inorganic compounds will be transferred by CCDC to the Inorganic Crystal Structure Database

(ICSD) after publication and will maintain the original deposition number(s). For all other crystallographic data that are not accommodated by the CCDC, authors are encouraged to deposit into a database according to instructions in the [Requirements for Depositing X-Ray Crystallographic Data](#) in addition to uploading the data in ACS Paragon Plus during manuscript submission as Supporting Information. Please indicate whether the other crystallographic data is intended for publication or for review only.

If restraints or constraints on nonhydrogen atoms or adjustments to the structure factors are used in the refinement of a crystal structure, these should be described in detail in the experimental section and their application justified. Data from complementary experiments should be made available to resolve any ambiguities arising from problems with a refinement.

Reporting of Data. The experimental section should describe how the crystals were obtained. The text as well as the experimental section should clearly state whether more than one independent molecule or any solvent molecules were found in the lattice. Any special molecular symmetry, such as an inversion center, should also be noted. Any disorder or partial (solvent) occupancy should be mentioned, together with how this was modeled or refined. Describe how any similarly sized ligands were distinguished (CO, NO, CN, etc.) and how any hydride ligands were located. With non-racemic compounds, the method by which the absolute configuration was assigned should be detailed.

An effort should be made to minimize the quantity of tabular material appearing in the printed text. Accordingly, the standard table of crystallographic data (data collection and refinement parameters, unit cell constants, space group information, final agreement factors) should be placed in the supporting information unless the contents are extensively discussed and analyzed in the text.

Depending upon the type of manuscript, abbreviated tables of bond lengths, bond angles, and other metrical parameters may be appropriate for the text. Such data may also be incorporated into figure captions.

Structural Representations. Color may be used in representations of crystal structures. The following Web sites offer guidance on atom coloring conventions: <http://jmol.sourceforge.net/jscolors> and http://en.wikipedia.org/wiki/CPK_coloring

Hydrogen atoms should not be depicted unless they play an important role in the structure (hydride ligand, hydrogen bonding, agostic interaction, etc.). Atoms refined anisotropically should never be depicted by spheres.

Computational Studies. Significant advances in computational facilities and the availability of electronic structure codes has led to a great increase in the number of computational papers being submitted to *Organometallics*. In addition to computational competence (level of theory, basis sets, etc.), for a manuscript to be appropriate for publication in *Organometallics* it must be strongly correlated to experimental data, address problems of broad interest to the organometallic community, and provide significant chemical insight.

Comparison of methods, studies of various levels of theory, basis set effects, etc., are considered to be technically oriented computational papers and are not encouraged. In addition, studies simply confirming results already present in the literature should be directed toward more specialized journals.

Authors should supply enough Supporting Information to reproduce the calculations or to make the results utilizable without repeating the calculations. This will normally include the following:

Description of specific programs and versions. If the author's own or a modified version of a commercially available program is used, it is required that the program/code/modification be made available to the scientific community (QCPE, publication in a computational journal, commercially, etc.). Policies in this regard are identical with those of several other ACS journals, as summarized in *J. Chem. Inf. Model.* **2006**, *46*, 937. A clear exposition of any nonstandard equations and algorithms used and, where feasible, tests of the codes in various limiting cases should also be provided.

Details of the computations. The computed molecular model should be described clearly, possibly with a ChemDraw figure. If the model is based on an experimentally known complex/reaction, any modifications (such as truncations) should be clearly described and justified. Final optimized coordinates and keywords are to be provided. For DFT computations, the choice of functional must be justified, or the validation of the functional provided. The choice of basis sets must be explicitly discussed, including any deviation from standard basis sets. Convergence criteria, integration parameters, active space definition in multireference calculations, and, for open-shell systems, the way in which spin states are handled should be mentioned explicitly. The exact definition of any applied numerical or symmetry constraint should be indicated.

Details of the computational results. When relevant to the results of the study, data such as absolute energies, gross orbital populations, atomic spin densities, etc., should be supplied. Where feasible, critical checkpoint/restart files should be saved and made available upon request.

Cartesian Coordinates. Cartesian coordinates of all molecules, intermediates, transition states, etc. that are part of the manuscript must be uploaded in a single file that is formatted for convenient viewing with widely available molecular modeling packages. The .xyz and .mol formats are accepted at this time. The .xyz format is the most basic and easily prepared from computational output.

The first line of the .xyz format file denotes the number of atoms in the molecule.

The second line of the file is a comments line, and should begin with a descriptive name of the molecule/structure consistent with the designation in the manuscript, and any other pertinent information selected by the author, such as total energy.

Next follow lines for each element in the molecule. Each line contains the element symbol followed by the x, y, and z coordinates in angstroms (Å) separated by spaces in free-field format (i.e. precise formatting not required). More information on the .xyz file format is available at <http://openbabel.sourceforge.net/wiki/XYZ>.

Multiple structures are placed directly end-to-end in the file.

The file name should have the extension ".xyz". A simple example with three molecules is shown below.

It is strongly recommended that authors view the structures in the file with a modeling program before uploading the file. The program **Mercury** (version 3.3 or later) is recommended for viewing and manipulating the multiple structures. The Cambridge Crystallographic Data Centre (CCDC) offers **Mercury** at no cost. Include the phrase “a text file of all computed molecule Cartesian coordinates in a format for convenient visualization” in the Supporting Information statement.

Example 3molecule.xyz file containing CO, CH₄, and H₂O created by text editing for CO and CH₄ and copy-and-pasting of coordinates from the output of a computation for H₂O (notice the variable spacing and variable number formats allowed in the free-field format):

```
2
carbon monoxide, electronic energy = -0.57115848 a.u.
C 0 0 0
O 0 0 1.1512345678
5
Methane, electronic energy = -0.70771290 a.u.
C 0 0 0
H .5 .5 .5
H -.5 -.5 .5
H .5 -.5 -.5
h -.5 .5 -.5
3
Water, electronic energy = -0.54307351 a.u.
H          -0.768340934      0.000000000      -0.106744877
O           0.000000000      0.000000000       0.513451800
H           0.768340934      0.000000000      -0.106744877
```

Language and Editing Services

A well-written paper helps share your results most clearly. ACS Publications' [English Editing Service](#) 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 [credit line](#) citing the original source. Authors are responsible for [obtaining written permission](#) 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 [Artwork Editing](#) and [Graphical Abstract](#) 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 [ACS Paragon Plus](#), 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

Organometallics authors are allowed to deposit an initial draft of their manuscript in a preprint service such as [ChemRxiv](#), 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. The preprint should be cited as a reference in the manuscript. Authors are discouraged from posting a revised version of the preprint, or for depositing the initial version of manuscript as a preprint, after the manuscript has been submitted and a decision is pending. Students may disseminate the final version of a thesis containing material in a submitted manuscript when previously filed as a publicly stated requirement for an undergraduate, masters, or Ph.D. degree posted on the official Web site of the degree-granting institution. All other prior/redundant publication or electronic posting with public or private access is forbidden without expressed permission from the Editor-in-Chief.

Editorial Policies

Information for Reviewers. *Organometallics* operates under a single-blind peer-review process. The quality of the articles published in the peer-reviewed chemical literature depends heavily on the thoroughness and rigor of the manuscript evaluations provided by reviewers. In addition, the editors of *Organometallics* rely on each reviewer's conscientiously prepared comments for helping maintain the high scientific standards of the journal. Please read the general information about [ACS Peer Review](#) and [ACS Publication Policies](#).

To help facilitate timeliness in the peer-review process, reviewers are expected to promptly respond to invitations to conduct a review and to promptly return their review before the deadline. The editors ask all reviewers to access the manuscripts they are reviewing and submit their reviews on the ACS Paragon Plus website; manuscript files will not be e-mailed or made available to reviewers by other means.

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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 [Table of Contents/Abstract Graphics](#) for specifications.

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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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