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## MANUSCRIPT SUBMISSION REQUIREMENTS CHECKLIST

- ☐ **Review Ready Submission:** ACS journals have simplified their formatting requirements (incl. references) in favor of a streamlined and standardized review-ready format for an *initial* manuscript submission. [Editorial](#)
- ☐ **Scope:** new and original experimental and theoretical research on molecules, macromolecules or materials that are catalytic in nature (exhibiting catalytic turnover). Additional scope information:
  - o Heterogeneous Electrocatalysis – [Editorial](#)
  - o Biocatalysis and Enzymology, Molecular Catalysis for Organic Synthesis, and Heterogeneous Photocatalysis – [Editorial](#)
- ☐ **Catalyst characterizations, comparisons to other catalysts:** [Editorial](#) (Preparing your manuscript for submission to *ACS Catalysis*) [Perspective](#) (Benchmarking)
- ☐ **Cover Letter:** must include a paragraph explaining why your manuscript is appropriate for *ACS Catalysis*, clearly indicating what key advance(s) are described in the work, and a statement confirming the manuscript has not been previously published by any of the authors and/or is not under consideration for publication in another journal at the time of submission.
- ☐ **Suggested Reviewers:** Submit names and email addresses of at least four scientists from different countries who could evaluate the work. These suggested reviewers must not be former mentors or mentees nor collaborators or coauthors from the past five years.
- ☐ **Disclosure of previous submissions:** If the manuscript was previously rejected by *ACS Catalysis*, provide the manuscript number and a detailed response to each reviewer's comments. If the manuscript was previously declined by any other journal, this must be disclosed; however, providing the journal name and additional information is optional.
- ☐ **Disclosure of prior publication & ACS Catalysis preprint policy:** Respond to the ACS Paragon Plus submission questions, "Has this manuscript in whole or in part been previously submitted to this journal? to another journal, either ACS or non-ACS?" [Disclosing Prior Submissions Editorial](#), [Preprint Policy Editorial](#), and [Outcomes of Disclosure Editorial](#)
- ☐ **Author list with affiliations:** must match between manuscript file and electronic entry at submission
- ☐ **Choose manuscript type:** Letter, Article, Perspective, Review, Viewpoint, Account, Correspondence, or Addition and Correction
- ☐ **Title and Abstract:** be clear and concise, reflect the emphasis and content of the paper. Titles and abstracts of manuscripts may not contain the words "New", "Novel", or "First"; "Superb", "Excellent", "Exceptional", "Outstanding" or other similar descriptive words discouraged unless rigorously supported by a thorough comparison with the state-of-the-art in the manuscript. [Superlative Scientific Writing Editorial](#)
- ☐ **5–8 Keywords:** these keywords will appear in the PDF version of the article and will be used as a search term in the HTML version of the article
- ☐ **Artwork Tables/Schemes/ Graphics:** Text should be clear and legible, ideally with Arial or Helvetica fonts, with fonts no smaller than 8 pt. ChemDraw must be in a specific format, [Chemistry is Beautiful Editorial](#). Figures must be mentioned in the text in consecutive order and number with Arabic numerals. Avoid inset figures.
- ☐ **References:** Include article titles in references [Editorial](#)
- ☐ **Safety:** authors must emphasize any unexpected, new, and/or significant hazards associated with the work
- ☐ **Table of Contents graphic:** required, dimensions of 3.33 in. width. (8.46 cm) and height, 1.87 in. (4.77 cm)
- ☐ **Cover Art** (optional): Authors may submit images to be considered for the cover (TIF, JPG, PNG or EPS files with a resolution of at least 300 dpi for pixel-based images). The image size is 6.9 in × 7.87 in., 17.5 cm × 20 cm, or 2100 × 2400 pixels.
  - ☐ **Supporting Information** (if any): must be included at the time of electronic submission. Include the heading "Supporting Information" followed by the manuscript title, author list, and affiliations. Tables, Schemes, and Figures should be written as Table S1, Figure S1, Scheme S1, etc.
- ☐ **Administrative considerations:** All papers must not be under consideration or published elsewhere; manuscripts will be screened with plagiarism software; information on whether the paper has been previously considered elsewhere must be provided; do not forget to list funding sources and ORCID

## SCOPE OF THE JOURNAL

*ACS Catalysis* is an interdisciplinary journal publishing original research on and at the interfaces of heterogeneous catalysis, homogeneous catalysis, and biocatalysis/enzymology. The journal is devoted to reports of new and original experimental and theoretical research on molecules, macromolecules or materials that are catalytic in nature (exhibiting catalytic turnover), and the catalysts should be characterized to the extent possible by turnover frequencies and fundamental kinetic parameters. Manuscripts that are essentially reporting data or applications of data are, in general, not suitable for publication in *ACS Catalysis*. While papers focusing on catalytic turnover (catalysis) will form the core of the journal, highly impactful papers characterizing catalytic materials or molecules (catalysts) will also be considered.

## MANUSCRIPT TYPES

*ACS Catalysis* publishes the following types of papers: Letters, Articles, Perspectives, Reviews, and Viewpoints. Accounts, Correspondence, and Additions and Corrections are also published.

**A. Letters** are short articles that report results whose immediate availability to the science and engineering community is deemed important. Letters are restricted to 2000 words or the equivalent (8 double-spaced typewritten pages of text and 4–5 figures). A brief abstract of less than 100 words should be included. Letters often will be complete publications, but follow-up publication may occasionally be justified when the research is continued and a more complete account of the work is deemed necessary. Special efforts will be made to expedite the reviewing and the publication of Letters. The time for proofreading the galley proofs is relatively short. For this reason, authors of Letters should ensure that manuscripts are in final, error-free form when submitted. A template for Letters is available (<http://pubs.acs.org/page/accacs/submission/templates.html>).

**B. Articles** should cover their subjects with thoroughness, clarity, and completeness but should be as concise as possible. Abstracts to Articles are typically limited to 300 words and should summarize the significant results and conclusions.

**C. Perspectives** are short reviews of recent developments in an established or developing topical area. Authors of perspectives are asked to provide a critical assessment of the field of interest, rather than a compilation and summary of literature reports. Perspectives will typically be 5–20 pages in length, depending on the topic being covered. Authors may be invited by the Editor to submit Perspectives. Unsolicited Perspectives will be considered, as well; however, authors interested in submitting a Perspective are strongly encouraged to contact the Editor prior to manuscript preparation and submission to seek conditional approval of the proposed review topic. One-page proposals should be sent to the Editor-in-Chief, Christopher Jones ([EIC@catalysis.acs.org](mailto:EIC@catalysis.acs.org)) for consideration.

**D. Reviews** are comprehensive, critical examinations of a selected topic, typically over a defined time period. Unsolved problems and emerging areas should be highlighted. A Review should consist of a maximum of 40 pages (approximately 65000 characters) of main text, footnotes, literature citations, tables, and legends. Most Reviews are expected to be substantially shorter in length, but the length will be dictated by the subject matter to some degree. Authors may be invited by the Editor to submit Reviews. Unsolicited Reviews will be considered, as well; however, authors interested in submitting a Review are strongly encouraged to contact the Editor prior to manuscript preparation and submission to

seek conditional approval of the proposed review topic. One-page proposals should be sent to the Editor-in-Chief, Christopher Jones ([EIC@catalysis.acs.org](mailto:EIC@catalysis.acs.org)) for consideration.

**E. Viewpoints** appear mostly as a result of an invitation from the Editor. Viewpoints may be general commentaries and tutorials of immediate interest to the broad readership. These articles normally will be in highly active research areas, and they are not intended to be reviews of the literature. The author will be asked to provide a clear, concise, and critical status report of the field as an introduction, and the author's own insights or contributions to the field should constitute the main body of the article. Viewpoints will typically range from 3 to 6 journal pages in length and have no abstract included. However, a Table of Contents graphic is required for this type of manuscript (see below for further information). Authors in highly active research fields of broad interest in catalysis are encouraged to propose Viewpoints to the Editor-in-Chief. Unsolicited Viewpoints will be considered, as well; however, authors interested in submitting a Viewpoint are strongly encouraged to contact the Editor prior to manuscript preparation and submission to seek conditional approval of the proposed topic. One-page proposals should be sent to the Editor-in-Chief ([EIC@catalysis.acs.org](mailto:EIC@catalysis.acs.org)) for consideration.

**F. Accounts** are reviews of a prominent catalysis researcher's scientific contributions, published to mark the researcher's retirement or other notable event/anniversary. They should include details of the researcher's career, including their scientific and technical influences and positions held, with the main body of the piece discussing the major new findings or advances he/she made over his/her career. In the majority of cases, these will be organized chronologically. Contributions are not written by the subject of the contribution, but are instead typically written by current or former associates of the scientist or engineer. Accounts adopt a format similar to Perspectives, being typically 6–20 journal pages in length and using figures, schemes, and tables where possible as well as photographs where appropriate. Note that permission must be obtained for use of all pictures and figures. Accounts will be published infrequently by the journal and are published on an invitation-only basis, though proposals may be sent to the Editor-in-Chief.

**G. Correspondence/Rebuttal.** Correspondence is a technical contribution providing, with supporting material, a respectful but alternative point of view to one that has appeared in *ACS Catalysis*. The author of the original publication may be invited to write a Rebuttal. The Correspondence and Rebuttal will appear in the same issue of the journal.

NOTE: Additions/Corrections, Retractions, and Expressions of Concern are included in the post-publication section (Publisher Content).

## 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, 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.
- [Sharing your research](#) with the public through ACS Publications open access program

## MANUSCRIPT PREPARATION

### Review Ready Submission

All ACS journals have simplified their formatting requirements in favor of a streamlined and standardized review-ready 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.
- A two-column manuscript template is available and can be used for manuscripts submitted to any ACS journal. Templates are not required but may be useful to approximate how an article will compose. For manuscripts with word count limits, authors are not required to fit content into a page limit based on the template.
- References can be provided in any style, but they must be complete, including titles.
- Supporting Information should be submitted as a separate file(s).
- Author names and affiliations on the manuscript must match what is entered into ACS.

### 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 Style Guide](#).

### 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.

Note: The cover letter is not the appropriate mechanism to declare a preference for assigned *ACS Catalysis* editor. Instead, those requests should be sent via email to the Editor-in-Chief ([eic@catalysis.acs.org](mailto:eic@catalysis.acs.org)) on the day prior to submission.

The cover letter to *ACS Catalysis* **must** contain the following elements. Please provide these elements in the order listed:

- A paragraph explaining why your manuscript is appropriate for *ACS Catalysis*. This paragraph should clearly indicate what key advance(s) is/are described in the work.
- If the manuscript was previously rejected by *ACS Catalysis*, provide the manuscript number of the rejected manuscript and a detailed response to each reviewer's comments.
- If the manuscript was previously declined by any other ACS journal, provide the name of the journal, the manuscript number, an explanation of the basis for the rejection, and a statement granting *ACS Catalysis* permission to obtain the Editor's decision letter and reviews for the declined manuscript. Please provide a detailed response to each reviewer's comments as outlined

in Section IV, Revised Manuscripts. If some version of the manuscript was previously submitted to a non-ACS journal, this submission **must** be noted in the cover letter, although further details regarding the review process are not required unless the authors choose to include them.

- A statement confirming the manuscript, or its contents in some other form, has not been published previously by any of the authors and/or is not under consideration for publication in another journal at the time of submission. Submission to a pre-print depository, such as ChemRxiv or bioRxiv is allowed, but must be noted in the cover letter.
- A description of any supporting information and/or Review-Only Material.
- The names and e-mail addresses of at least four possible reviewers. These suggested reviewers must not be former mentors or mentees nor collaborators or coauthors from the past five years. Ideally, two or more suggested referees will work in different countries from the authors, when possible. Non-preferred reviewers may be denoted, along with a reason for their designation.

## Manuscript Text Components

### Title

Titles should clearly and concisely reflect the emphasis and content of the paper. Titles are of great importance for current awareness and information retrieval and should be carefully constructed for these purposes. **Titles of manuscripts may not contain the words “New”, “First”, or “Novel” nor any part number or series number without permission from the Editor. Additionally, “Superb”, “Excellent”, “Exceptional”, “Outstanding” or other similar descriptive words, are strongly discouraged.**

### Author List

Bylines should include all those who have made substantial contributions to the work. To facilitate indexing and retrieval and for unique identification of an author, use first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and last names (e.g., J. Robert Smith). At least one author must be designated with an asterisk to indicate the person to whom readers may send correspondence. There should be no more than three corresponding authors per paper. Deceased persons who meet the criterion for inclusion as co-authors should be so included, with a footnote indicating the date of death.

### Institution Address

The author affiliation(s) listed should be the institution(s) where the work was conducted. If the present address of an author differs from that at which the work was done, the current address should be given in a footnote. The e-mail address(es) of the corresponding author or authors must also be provided as a separate line below the institution addresses.

Many Funders and Institutions require that institutional affiliations are identified for all authors listed in the work being submitted. ACS facilitates this requirement by collecting institution information during manuscript submission under Step 2: Authors and Affiliations in ACS Paragon Plus.

### Abstract

All Articles, Letters, Perspectives, and Reviews must be accompanied by an abstract, including an Abstract (TOC) graphic, which should state briefly the purpose of the research (if this is not contained in the title), the principal results, and major conclusions. Abstracts of manuscripts may not contain the words “superb”, “excellent”, “exceptional”, “outstanding”, or other similar descriptive words unless rigorously supported by a thorough comparison with the state-of-the-art in the manuscript. Like manuscript titles, **the words “New”, “First”, or “Novel” are also generally disallowed in the abstract.**

## Keywords

All Articles, Letters, Perspectives, and Reviews must be accompanied by 5–8 keywords. These keywords will appear in the PDF version of the article and will also be used as a search term in the HTML version of the article.

## Text

All sections of the paper must be presented in a clear and concise manner. Authors should include an introductory statement outlining the scientific motivation for the research. The statement should clearly specify the questions for which the answers are sought as well as the connection of the present work with previous and current work in the field. In both Letters and Articles, the introduction should be a separate section of the paper. In the discussion section, the author should discuss the significance of his/her observations, measurements, or computations. Conclusions of manuscripts may not contain the words “superb”, “excellent”, “exceptional”, “outstanding” or similar descriptive words unless the claim is rigorously supported by a thorough comparison with the state-of-the-art in the manuscript. The author should also point out how they contribute to the scientific objectives indicated in the introduction. Tabulation of experimental results is encouraged whenever it leads to a more effective presentation or economical use of space. Authors are encouraged to make extensive use of the Supporting Information format, because this material is now widely available on the Web at <http://pubs.acs.org>.

**Plagiarism.** Manuscripts must be original with respect to concept, content, and writing. It is not appropriate for an author to reuse wording from other publications, including one’s own previous publications, whether or not that publication is cited.

**Figures.** All figures must be mentioned in the text in consecutive order and must be numbered with Arabic numerals and placed in the text near the point of first mention. Figures should use Arial or Helvetica fonts, whenever possible. A caption giving the figure number and a brief description, preferably only one or two sentences, must be included. The caption should be understandable without reference to the text. It is preferable to place a symbol key or graphical legend in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork. Authors are required to ensure that similar figures have similar resolution and quality (all black and white figures should have resolution similar to each other; all color figures should have resolution similar to each other). See the section under “Artwork” for details.

**Schemes.** Sequences of reactions are called schemes and should be numbered consecutively with Arabic numerals and placed in the text near the point of first mention. Schemes may have brief titles describing their contents and footnotes, if needed, for further detail.

**Charts.** Groups of structures that do not show reactions are called charts and should be numbered consecutively with Arabic numerals and placed in the text near the point of first mention. Charts may have brief titles describing their contents and footnotes, if needed, for further detail.

**Tables.** Tables may be created using a word-processor’s text mode or table format feature. The table format feature is preferred. Ensure that each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row.

Tables should be numbered consecutively with Arabic numerals and placed in the text near the point of first mention. 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 as narrative, when many numbers must be presented, or when more meaningful interrelationships 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.

Define nonstandard abbreviations in footnotes. Footnotes in tables should be given letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column. If a reference is cited both in the text and in a table, a lettered footnote which refers to the numbered reference in the text should be placed in the table.

In setting up tables, authors should keep in mind the type area of the *ACS Catalysis* page (17.8 cm × 23.5 cm) and the column width (8.5 cm) and should make tables conform to the limitations of these dimensions.

## 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 description of each file is required, and the paragraph and descriptions should be placed at the end of the manuscript before the list of references. The appropriate format is as follows:

**Supporting Information.** Brief descriptions in nonsentence format listing the contents of the files supplied as Supporting Information.

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.

## Data Requirements

### Compound Characterization, Experimental and Computational Data

Authors are required to provide sufficient information (as described in more detail below) to establish the identity of a new compound, its purity, and its yield. Sufficient experimental details must also be included to allow another researcher to reproduce the synthesis. *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. Characterization data and experimental details must be included in either the paper or the Supporting Information. Guidelines for reporting NMR data are available online at <http://pubs.acs.org/page/4authors/tools/index.html>. Note that, when possible, unambiguous peak assignments should be given for all NMR spectra.

### ***Guidelines for Characterization of Organometallic and Inorganic Compounds.***

#### (a) Routine Compounds

Compounds in this category are those that have literature precedent. Sufficient data must be provided to identify and verify the structure of such compounds, and the original preparation should be cited in either the Experimental Section or the Supporting Information. When possible, representative spectra should be provided in the Supporting Information.

**(b) Novel or Unexpected Compounds**

Compounds in this category are those that either (i) exhibit an unprecedented type of structure, or (ii) are obtained by unexpected reaction. Such compounds require more detailed characterization to ensure their validity and purity. In the majority of cases, evidence for elemental constitution must be provided by elemental analysis. If accurate elemental analysis data are not possible, a clear statement to this effect must be included within the text of the manuscript and other methods to establish purity and identity given (e.g., mass spectrometry data and representative NMR data should be provided in the Supporting Information). Please note that, in many cases, spectroscopic data are insufficient to establish purity owing to the presence of undetectable species. In addition to elemental analysis and/or mass spectrometry data, spectroscopic techniques should be used to provide sufficient characterization (including NMR, IR, UV–vis or EPR spectroscopy). To the extent possible, resonances from NMR data should be assigned to specific chemical functionality. While an X-ray diffraction structure is not considered definitive proof of elemental composition, it is acceptable evidence for composition, providing that the results of other physical methods concerning the characterization are conclusive.

**(c) Solid State Materials**

Compounds in this category are those that have no existence in solution. Solid state materials, such as heterogeneous catalysts, must be characterized in such a way as to sufficiently describe their structure and composition. Atomic ratios and elemental compositions must be provided for solid state materials. X-ray diffraction data should be provided for crystalline materials.

**(d) Compounds That Have Not Been Isolated**

Compounds that have not been isolated in pure form (e.g. reaction intermediates, intractable mixtures, or unstable species) may be published. However, in these circumstances, an explicit statement must be given in the paper (not only in the Supporting Information) indicating that the compounds have not been isolated. Only in exceptional circumstances will a paper be published in which none of the new compounds reported has been isolated and fully characterized.

**(e) Purity and Yield**

The yield and purity of all molecular species must be reported, including the methods used to determine them. The yield of a compound obtained in an NMR tube reaction should be determined using an internal standard. Similarly, internal standards and/or calibration curves must be employed in determining GC yields.

***Guidelines for Characterization of Organic Compounds***

**(a) Sample Quality**

For new substances, evidence of the homogeneity of the purified sample should be included. Elemental analysis is sufficient. If no analysis was performed, then sufficient other evidence (for example,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, HPLC, GLPC, gel electrophoresis, etc.) must be included as figures in the Supporting Information.

**(b) Molecular Weight**

Evidence of molecular weight should be provided, especially if elemental analysis is not performed. Low-resolution MS data under conditions that minimize fragmentation are acceptable. If there is a specific need to distinguish alternative formulas with the same molecular mass (within one amu), then HRMS data are necessary.

(c) Miscellaneous

Numerical listings of characteristic spectroscopic data should be included to support assigned structures, changes in functionality, unusual chromophores, etc. Methods of purification used to prepare samples for characterization should be described. For crystalline samples, information about the method of crystallization should be included (solvents; mp; etc.). For non-racemic, chiral substances, data to allow correlation of absolute configuration should be given, preferably including  $[\alpha]_D$  values. If correlation data are provided based on HPLC or GLPC methods, then retention times for both enantiomers must be provided, together with solvent and flow rate information, and identification of the chiral support.

(d) Intermediates on Solid Phase; Combinatorial Chemistry

Validation of methods and characterization of new substances in a statistically significant sampling should be provided. Resin-bound intermediates need not be characterized if acceptable end product quality (as defined in a–c above) is demonstrated.

### ***Kinetic and Equilibrium Data***

The reporting of kinetic data and equilibrium binding data for proteins, nucleic acids, and other species should preferably include a description of the identity of the catalyst or binding molecule, its origin, purity of composition, and any modifications, such as mutations, post-translational modifications, or other modifications made to facilitate expression and purification. The method of assay and the exact experimental conditions of the assay should be provided as a reference to previous work, with or without modifications, or fully described if a new assay. Conditions essential to reproduce the results, such as the temperature, pH, and pressure (if other than atmospheric) of the assay should be included. Terms such as “not detectable” (ND) should be avoided. Instead, an estimate of the limit of detection based on the sensitivity and error analysis of the assay should be provided. Authors are referred to the STREND A (Standards for Reporting Enzymology Data) Commission of the Beilstein Institut (<http://www.strenda.org/documents.html>) for an example of detailed guidelines.

### ***Structural and Sequence Data for Proteins and Nucleic Acids***

Atomic coordinates and structure factors for proteins determined by X-ray crystallography and coordinates determined by NMR should be deposited with the Protein Data Bank, Research Collaboratory for Structural Bioinformatics at Rutgers University. Theoretical model depositions are no longer accepted for inclusion in the PDB archive. Structures of nucleic acids should be deposited with the Nucleic Acid Database. It is the responsibility of the author to obtain a file name (PDB ID or NDB ID) for the molecule; the file name must appear in the published manuscript. DNA and amino acid sequences should be deposited in a public sequence repository such as DNA DataBank of Japan (DDBJ), the European Nucleotide Archive (ENA), or GenBank at National Center for Biotechnology Information. A manuscript will be sent out for review without the file name only after receipt from the submitting author of a written statement that the coordinates will be deposited. If a file name has not yet been obtained upon acceptance of a paper, it must be added in proof. Atomic coordinates and structure factors for all structures must be released immediately upon publication of the paper.

### ***Single Crystal Diffraction Data***

Manuscripts reporting the determination of one or more structures by X-ray diffraction must adhere to the following requirements:

**Abstract.** The abstract may summarize geometric features of unusual interest but should not contain unit cell parameters.

**Main Body of Manuscript.** Tables of essential interatomic distances and angles are not required but may be submitted (metric information for standard structural components should not be included).

For structures with anisotropically refined atoms, a figure displaying the thermal ellipsoids should ordinarily be presented; a spherical-atom representation may be substituted if necessary for clarity. If a spherical atom view is chosen for the manuscript, a thermal ellipsoid figure should be included in the Supporting Information. In cases when intermolecular interactions are relevant to the discussion, a view of the unit cell may be included.

An Article should list for each structure the formula, formula weight, crystal system, space group, color of crystal, unit cell parameters, temperature of data collection, and values of *Z*, *R*, and GOF; a brief description of data collection, and solution and refinement of the structure, should be placed in the Supporting Information. Tables of atom coordinates and thermal parameters will not be printed.

### ***CIF Submission Instructions***

If single crystal X-ray structures are reported, authors are required to submit X-ray crystallographic data to be published as Supporting Information. The information required for each structure should be submitted in the electronic Crystallographic Information File (CIF) format. Such files should be submitted electronically as described below.

CIFs must be uploaded at the same time the manuscript is submitted via the Web, with the file designation Supporting Information for Publication. The CIF for each structure should be uploaded as a separate Supporting Information file. CIFs should be saved in the text-only (plain ASCII) format, with a .cif extension before being submitted. No information other than the CIF itself should be included inside the file. CIFs may NOT be furnished as Microsoft Word, Corel WordPerfect, or PDF files.

Before submission, CIFs must be checked using the CheckCIF utility on the Web at <http://checkcif.iucr.org/>. A copy of the output should be retained in case it is requested by an Editor. Authors with appropriate software may alternatively use IUCRVAL or the CHECK validation tool in PLATON.

If CIFs are not available, the required data should be furnished in neatly formatted tables with informative titles that identify the name or the structure number of the compound.

### ***Powder Diffraction Data***

No special instructions apply to the use of X-ray powder diffraction in a routine manner to characterize heterogeneous catalysts. However, for new crystalline materials or for crystalline materials previously uncharacterized by this technique, specific guidelines are given here. In such cases, data from X-ray powder measurements should be accompanied by details of the experimental technique: source of X-rays, the radiation, its wavelength, filters or monochromators, camera diameter, the type of X-ray

recording, and the technique for measuring intensities. In cases of unindexed listing of the data, the  $d$  spacings of all observed lines should be listed in sequence, together with their relative intensities. In cases where filtered radiation is used, every effort should be made to identify residual  $\theta$  lines. Where resolution into  $\alpha_1$ – $\alpha_2$  doublets occurs, the identification of the  $d$  spacing for each line as  $d\alpha_1$ ,  $d\alpha_2$  gives a measure of the quality of the diffraction pattern. When an indexing of the data is offered, the observed and calculated  $1/d^2$  values should be listed along with the observed relative intensities (it is superfluous to give  $d$  spacings in this instance). All calculated  $1/d^2$  values should be listed (exclusive of systematic absences), to the limit of the data quoted. If possible, the crystal system should be specified. Possible space groups may also be listed if the data warrant it. Relevant information about the specimen used should be included.

### ***Mechanistic Proposals***

To support mechanistic proposals, characterization of intermediate species with multiple spectroscopic methods should be done, when possible, and/or adequately supported by theoretical calculations. Furthermore, mechanistic proposals should be adequately backed by experimental data or experimentally calibrated theoretical methods.

### ***Computations***

When computational results are an essential part of a manuscript, sufficient detail must be given, either within the paper or in the Supporting Information, to enable readers to reproduce the calculations. This includes data such as force field parameters and equations defining the model (or references to where such material is available in the open literature). If the software used for calculations is generally available, it must be properly cited in the References. References to the methods upon which the software is based must also be provided. Results obtained from methods or parameters that are not adequately described in the manuscript or in the literature are not acceptable for publication. Authors who report the results of electronic structure calculations are requested to provide as Supporting Information the geometries (either as Cartesian coordinates or Z matrices) of all the stationary points whose relative energies are given in the manuscript. The absolute energies in hartrees that are computed at these geometries should not be given in the manuscript but should be included in the Supporting Information. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states.

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(1) As drawing settings select:

chain angle	120°
bond spacing	18% of width
fixed length	14.4 pt (0.508 cm, 0.2 in.)
bold width	2.0 pt (0.071 cm, 0.0278 in.)
line width	0.6 pt (0.021 cm, 0.0084 in.)
margin width	1.6 pt (0.056 cm, 0.0222 in.)
hash spacing	2.5 pt (0.088 cm, 0.0347 in.)

(2) As text settings select:

font	Arial/Helvetica
size	10 pt

(3) Under the preferences choose:

units	points
tolerances	5 pixels

(4) Under page setup choose:

Paper	US Letter
Scale	100%

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## Appendix 1: PREPARING FOR SUBMISSION

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- Color art 300 dpi

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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 its contents

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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.

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