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Last updated: December 18, 2024 View the latest guidelines online

Manuscript Submission Requirements Checklist

- **Submit with Fast Format**: ACS journals have simplified formatting requirements with a streamlined and standardized review-ready format for an *initial* manuscript submission. Include article titles in references.
- **Cover Letter**: must include a paragraph explaining why your manuscript is appropriate for *ACS Organic & Inorganic Au*, clearly indicating what key advance(s) are described in the work relative to the state-of-the-art, 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 six scientists from at least three different countries who could evaluate the work. These suggested reviewers must not be former mentors or mentees nor collaborators or co-authors from the past five years.
- **Disclosure of previous submissions**: If the manuscript was previously rejected by *ACS Organic & Inorganic Au*, provide the manuscript number and a detailed response to each reviewer's comments. If the manuscript was previously declined by any other journal, even without external peer review, this must be disclosed; however, providing the journal name and additional information is optional.
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- **Author list with affiliations**: List of authors, order of authors, author affiliations, and manuscript title must be the same on all pieces of the submission and match the electronic entry at submission.
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- **References**: Include article titles in references.
- **Safety**: Authors must emphasize any unexpected, new, and/or significant hazards associated with the work.
- **Table of Contents graphic**:

- required, dimensions of 3.25 inches by 1.75 inches (approx. 8.25 cm by 4.45 cm)
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- **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. All pages of the PDF Supporting Information should be numbered consecutively. Copies of all related works that are “in press”, “accepted”, or “submitted” for publication or in the late stages of preparation must be uploaded as Supporting Information for Review Only at the time of submission. References that are only available online should be cited by the Digital Object Identifier (DOI).
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Scope of the Journal

ACS Organic & Inorganic Au is an open access journal that publishes original experimental and theoretical/computational studies on organic, organometallic, inorganic, crystal growth and engineering, and organic process chemistry. Short letters, comprehensive articles, reviews, and perspectives are welcome on topics that include:

Organic chemistry:
- Physical and theoretical organic chemistry, including mechanistic studies
- Natural products isolation, identification, and synthesis
- New synthetic methodology, including single or multistep reactions and total synthesis
- Bioorganic and medicinal chemistry
- Materials science: Polymer chemistry and studies on functional molecules and systems

Organometallic chemistry:
- Synthesis, structure, bonding, chemical reactivity, and reaction mechanisms for a variety of applications, including catalyst design and catalytic processes
- All aspects of main-group, transition-metal, and lanthanide and actinide metal chemistry
- Synthetic aspects of polymer science and materials science
- Bioorganometallic chemistry

Inorganic Chemistry:
- Coordination chemistry involving transition metals, lanthanides, and actinides
- Main-group and organometallic chemistry
- Bioinorganic chemistry
- Catalyst design and catalytic processes
- Solid-state/materials/nanoscale chemistry

Organic Process Chemistry:
- Practical applications of organic chemistry that enable the safe, environmentally benign, and ultimately economical manufacturing of organic compounds at large-scale

Crystal Growth and Engineering:

- Organic, inorganic, hybrid solids, biological substances (e.g., biomineralization)

Manuscript Types

Articles should report a significant advance in a subfield of chemistry, being characterized by the editor and referees as an advance representing the top 10% of articles published annually in that field. Articles must be of high scientific quality, originality, significance, and conceptual novelty. Articles that mainly expand findings that were previously published as Letters in *ACS Organic & Inorganic Au* or elsewhere and that only incorporate experimental data, without greatly expanded scope and without providing new insights or conceptual breakthroughs, will be declined or recommended for Manuscript Transfer to specialized journals. Similarly, articles that are mainly routine extensions of previously published related work will be declined or recommended for Manuscript Transfer to specialized journals.

Use of the template for Articles is strongly encouraged but is not required. If an author chooses not to use a template to prepare an Article, only Times and Symbol fonts and 1.5 or double line spacing should be used. Other fonts may cause problems when the PDF files used for review are created. Also, if the template is not used, the document mode or its equivalent in the word-processing program should be used; i.e., files should not be saved in “Text Only” (ASCII) mode. If a non-Western version of word- processing software is used to prepare the manuscript, the file should be saved in rich-text format (RTF).

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.

Letters are short publications that report results whose immediate availability to the science and engineering community is deemed important. A Letter must convey the scientific findings concisely in a brief abstract, main text, and graphical elements as determined by word count not exceeding 2,200 words, including titles/footnotes/captions of approximately five graphics (typically 2 inches long in a single column). References are not included in word count to allow article titles to be included at submission. To calculate word count within the word processing application, select all text from abstract through end of main text (excluding title, authors, affiliations, and content after main text) and view the word processor’s word count data. Letters exceeding the word count limit must be shortened before acceptance. Note: *ACS Organic & Inorganic Au* encourages submission of Letters ranging from approximately 1,200-2,200 words (equivalent to 2-4 formatted journal pages), with more concise submissions appropriate for the most urgent new findings of exceptional significance.

All graphics and tables must be placed near the point of first mention in the text of the manuscript (not grouped at the end of the document) and must be sized according to current guidance. Long notes are not permitted in the References section; information not directly germane to the Letter can be included as Supporting Information. Letters can be complete publications, but follow-up publication may be justified when the research is continued and a more complete account of the work is deemed necessary, especially for the most urgent concise Letters noted above. 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.

Reviews are topical, forward looking, and of general interest to the readership. Length is flexible

(6–20 or more pages). A good review critically evaluates existing work of multiple groups in a field or across disciplines, provides a logical organization, and makes the material more easily available to those not expert in the area through clear text and figures. Reviews should lay out the challenges and opportunities that lie ahead. Reviews should contain an abstract and appropriate references. The use of graphics to illustrate key concepts is strongly encouraged. Reviews include a graphical Table of Contents entry. Reviews also include ~8–10 keywords and a vocabulary section in which 5–7 terms extracted from the text are defined in one or two sentences.

Perspectives are personal reviews of a field or area by one or a small team of authors, and they are focused rather than comprehensive. Perspective authors are asked to assess the current status of the field with an emphasis toward identifying key advances being made or those advances that are needed, and with an eye to the future. An *ACS Organic & Inorganic Au* Perspective should touch base with the current literature, including key contributors and references, but will primarily serve to inspire and help direct future research efforts. Authors may be invited by the Editor to submit Perspectives. Perspectives may not exceed 10,000 words in abstract, main text, and graphical elements.

Authors interested in submitting a Review or Perspective are strongly encouraged to contact the Editor prior to manuscript preparation and submission, to seek conditional approval of the proposed topic. Authors interested in contributing a Review or Perspective should email the Editor, Geraldine Masson (masson-office@orginorgau.acs.org), providing a single document that includes the following information for consideration:

1. Proposed Review or Perspective title
2. Corresponding author names, affiliations, and websites
3. A short (~400 word) description of the focused topic
4. A list of 5-10 lead references that will form the foundation of the manuscript
5. A list of recent review articles published on this topic, written by the submitting authors or others, and an explanation of how the proposed review will differ in focus and advance the literature on the subject.

Correspondence/Rebuttal. Correspondence is a technical contribution providing, with supporting material, a respectful but alternative point of view to a publication that has appeared in *ACS Organic & Inorganic Au*. 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, when possible.

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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.

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- 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).

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

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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 letter must provide the corresponding author’s name, title, affiliation, and e-mail address. All Editorial correspondence concerning receipt, status, review, revision, and publication of a manuscript will be sent only to one person who has been designated as the corresponding author during the evaluation period. The corresponding author is responsible for communicating the manuscript status to all co-authors of the manuscript and for obtaining the co-authors’ assent to

any substantial changes of content or interpretation made during revision. While a cover letter with designate a single corresponding author who serves as the primary contact during the submission and review process, additional corresponding authors may be designated with asterisks in collaborative manuscripts, with the number of corresponding authors not to exceed three.

The cover letter must include a paragraph explaining why your manuscript is appropriate for *ACS Organic & Inorganic Au*. This paragraph should clearly indicate what key advance(s) is/are described in the work. The letter may suggest the name of an appropriate *ACS Organic & Inorganic Au* Associate Editor. However, manuscript assignment to an Associate Editor is ultimately at the discretion of the Editor-in-Chief. Non-preferred Associate Editors and reviewers may be denoted in the cover letter, along with a reason for their designation.

The cover letter should provide explicit assurance that the manuscript is not under consideration for publication and has not been published elsewhere. Please note any submission to a preprint server such as ChemRxiv, bioRxiv, or arXiv 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.

Manuscript Text Components

Title. Titles should clearly and concisely reflect the emphasis and content of the manuscript. 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” or “Novel” nor any part number or series number without permission from the Editor. Claims of precedence should not be made in a title, so use of “First” in titles for this purpose is prohibited. Additionally, “Superb”, “Excellent”, “Exceptional”, “Outstanding” or other similar descriptive words, are strongly discouraged. Acronyms and abbreviations are not permitted in manuscript titles, unless they are broadly familiar to readers in all disciplines of chemistry. Titles should not be phrased as a question.

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 or first initials (e.g., Jody R. Smith), second names, and last names (e.g., J. Riley Smith). Do not use only initials with surnames (e.g., J. R. Smith). Deceased persons who meet the criteria for inclusion as coauthors should be included, with an Author Information note indicating the date of death. Do not include professional or official titles or academic degrees. At least one, or optionally more than one but fewer than four authors must be designated with an asterisk as the author(s) to whom reader correspondence regarding the published manuscript may be addressed.

The full names and e-mail addresses of all co-authors must be provided on the Authors & Institutes page upon submission of the manuscript in ACS Paragon Plus. Use of ORCID identifiers is encouraged.

Addition or deletion of an author or authors after submission of the manuscript requires justification from the corresponding author and is subject to approval by the Editor.

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Abstract. All Articles, Letters, and Perspectives) must be accompanied by an abstract, including an Abstract (TOC) graphic, which should state briefly the purpose of the research, 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. The abstract should not generally exceed 200/300 (Letter/Article) words. Pasting the abstract in the text box on the Web submission page does not replace the need for including an abstract in the manuscript document.

Keywords. All Articles, Letters, and Perspectives 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 (Articles). The first paragraphs of an Article should explain the motivation for and import of the work, where it fits in the development of the field and of chemistry, and perhaps why it should be of interest to chemists in other areas. It should be possible to do this without excessively increasing the length of the Article. Extensive reviews of the literature cannot be accepted. Thoughtful use of schemes and figures (with well-composed captions) is recommended, so that even casual browsers can discern the nature of the work. Well-known procedures should be designated by name, or literature references to them should be given. Experimental results are of lasting value and should be clearly and logically presented in a separate section. Standard Article format must be used for preparing a manuscript for submission as an Article, including section headings and a proper Introduction, a complete Experimental Section (unless placed in the Supporting Information), Results, and Discussion. The addition of a Conclusion section at the end of the manuscript, which briefly summarizes the principal conclusions of the work, is recommended. If desired for clarification, section headings may be given Arabic numbers and subsections numbered in decimals (e.g., subsection 2.1 and subsection 2.2).

Text (Letters). Section headings (Introduction, Experimental Section, Conclusion, etc.) should not be used in a Letter.

Safety. Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. For each manuscript that reports experimental procedures, authors must include an affirmative statement about safety in the Experimental Section of the full article or the main text of a Letter. Further information may be included or re-introduced in the Supporting Information.

Data Availability Statement. A Data Availability Statement is required for all peer-reviewed articles and is not required for the following non-peer-reviewed articles: Addition/Correction, Editorial, Expression of Concern, or Retraction. The ACS Research Data Policy provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Appendices. Appendix sections must be placed in the Supporting Information.

Dedications. All dedications must appear in the Acknowledgment section and are subject to

approval by the Editor.

Abbreviations. Acronyms and abbreviations that are not broadly familiar to readers in all disciplines of chemistry should be introduced in parentheses following the full term on its first appearance in the text. Do not include a separate Abbreviations list.

Acknowledgment. Dedications and notes acknowledging financial or professional assistance to the conduct of research or indicating presentation at a meeting should be brief and placed in the Acknowledgment section.

Author Information Notes. The e-mail address(es) of the corresponding author or authors must be provided as a Corresponding Author note. Present addresses for individual authors that differ from the address(es) at which the work was done should be given in a Present Address(es) note.

Statements about author contributions to the work or equal contributions of work should be included as a separate statement.

References and Footnotes. *All the references and footnotes must be placed together in a list at the end of the manuscript text.* In the Web edition, many of them will have links to other Web resources, such as the corresponding abstracts in *Chemical Abstracts* and the full text from other American Chemical Society journals. Because of this electronic linking, and to aid scientific research, *it is crucial that authors verify the accuracy of all references.*

Unnecessarily long lists of references should be avoided, and excessive self-citation is not permitted. However, authors must reference all previous publications in which portions of the present work have appeared. Each literature reference should be assigned one number and placed in the text as a superscript Arabic numeral. Footnotes to the text should be combined with references and numbered in ordinal sequence. Long footnotes should be avoided in Articles and are not permitted in Communications; additional data and peripheral discussion should be placed in the Supporting Information rather than in footnotes.

Bibliographic references to classified documents and reports or references to unpublished materials that are not generally available to the scientific public should not be used. Authors must obtain written permission from any person whose work is cited as a personal communication, unpublished work, or work in press. Copies of letters of permission and documentation should be appended to the cover letter file. If the manuscript is accepted but the necessary permissions have not been received, the Editor will ask the author to remove the reference(s) and dependent text.

List submitted articles as “in press” only if they have been formally accepted for publication. Otherwise, use “unpublished work” with the name of the place where the work was done and the date. For work published online (ASAP, in press), the DOI should be furnished in addition to the author name(s), article title, journal name, and year. DOI is an accepted form of citation before and after the article appears in an issue.

Example of a journal reference:

Yue, Q.; Liu, W.; Zhu, X. n-Type Molecular Photovoltaic Materials: Design Strategies and Device Applications. *J. Am. Chem. Soc.* **2020**, 142*,* 11613–11628.

Example of an in-press journal reference:

Ham, J. S.; Park, B.; Son, M.; Roque, J. B.; Jurczyk, J.; Yeung, C. S.; Baik, M.-H. ; Sarpong, R. C–H/C–C Functionalization Approach to N-Fused Heterocycles from Saturated Azacycles. *J. Am. Chem. Soc.* **2020**, DOI: 10.1021/jacs.0c04278.

Example of a reference to a book with no editors:

Desiraju, G. R.; Vittal, J. J.; Ramanan, A. *Crystal Engineering: A Textbook*. World Scientific Publishing Co Pte Ltd: Singapore, 2011.

Example of a reference to a book with editors:

Byrn, S. R.; Stowell, J. G. Impurities in Drug Substances and Drug Products. In *Validation of Active Pharmaceutical Ingredients*; Berry, I.R., Harpaz, D., Eds.; CRC Press: Boca Raton, 2001; pp 271–292.

Authors should consult the ACS Guide to Scholarly Communication for the appropriate style to use in citations of journal articles, books, and other publications. In literature references, article titles must be included and journal abbreviations should be those used in the *Chemical Abstracts Service Source Index (CASSI)*.

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: ^{1}H 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.

ACS Organic & Inorganic Au applies ACS Research Data Policy **Level 1**, meaning the journal encourages all authors to publicly share all the data underlying the results reported in the paper, preferably via archiving in an appropriate public repository. Authors are also encouraged to provide a Data Availability Statement describing the public availability of the data supporting the

article’s conclusions. Publicly available data sets should be cited appropriately.

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

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.

Data Requirements

Compound Characterization, Experimental and Computational Data

Please see the ACS Research Data Guidelines for more information on data requirements. 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. The Experimental Section should describe methods in sufficient detail to permit repetition of the work by others. 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. Note that, when possible, unambiguous peak assignments should be given for all NMR spectra.
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.

General Experimental Methods. A General Experimental Methods paragraph may be optionally provided to document procedures (such as purification methods, solvent removal, and spectroscopic and chromatographic analyses) that are common to most of the individual procedures, and it should be placed at the beginning of the Experimental Section.
Sources of stationary phases for chromatography and supports for solid phase synthesis may be identified. Sources of reactants, reagents, and solvents should *not* be identified except for (1) starting compounds that are unusual or not widely available; (2) materials for which the author has reason to suspect that the source is critical to the outcome of an experiment; and (3) catalysts. In the latter two cases, available purity information should be reported. Experiments involving a catalyst, enzyme, or reagent that is neither commercially available nor prepared by a fully described or cited nonproprietary method may not be reported.

Synthesis Experiments. Synthesis procedures for new compounds should be accompanied by yields and the most important product characterization data. Graphic structures of synthesized products (but not reaction schemes or other graphics) may accompany the characterization data listings. When known compounds have been prepared, procedures that were reported in the Experimental Section or Supporting Information of a previous publication should be cited but not reported in detail unless they have been modified.
Fully characterized compounds should have bolded compound names and structure numbers as the titles of the paragraphs in which their preparation, isolation, purification, and properties are described. Intermediates in multistep sequences that have not been purified and fully characterized should not have their names bolded; their preparation and partial characterization should be described as a step in the synthesis of a fully characterized bold-titled compound.
Reactant, reagent, and catalyst quantities should be given in both weight and molar units. Reaction solvent volumes and reaction times should be reported. 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.

All reported yields should represent weighed amounts of isolated and purified products and must be reported in the Experimental Section as both weights and percentages. 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. When a series of related compounds has been prepared using substantially the same procedure, it is usually sufficient to present a single representative example. If instead a general synthesis procedure reporting only relative molar quantities (as equivalents) is presented, the relative solvent volume also needs to be reported (as the molarity of the limiting reactant or reagent in the reaction mixture). If the several examples were not all conducted at the same molar scale, the paragraphs describing the individual products should include, along with the yields, the weights and molar amounts of the limiting reactants, for example, "yield 177 mg (78%) from 198 mg (0.66 mmol) of 3d."

When chromatographically or spectroscopically determined conversions of starting material to product are presented in a table documenting a synthetic transformation using a range of starting materials, reagents, or reaction conditions, a column heading or footnote should identify which quantity is being reported. The isolation and purification of the products for several representative examples should be reported in the Experimental Section, and the yields of isolated product for those examples should be included in the table.

Manuscripts that illustrate a new or modified synthetic method with multiple examples conducted on a submillimolar scale should include one or more examples carried out on a larger scale to demonstrate the practical utility of the method as a synthetic tool.

When preparative chromatography is used for product purification, both the stationary phase and solvent should be identified. Where different solvent mixture ratios, or different gradient elution schemes, have been used for purifying the members of a series of related compounds whose preparation is described with a single example or a single general procedure, the mixture composition or gradient scheme should be individually reported for each compound.

For reactions that require heating, identify the temperature and heat source (oil bath, heating mantle, etc.) or the model and manufacturer number if a device is used, e.g. a microwave or sonicator. Reports of syntheses conducted in microwave reactors must indicate whether sealed or open reaction vessels were used, how the reaction temperature was monitored (external surface sensor or internal probe type), and the temperature reached or maintained in each experiment. *ACS Organic & Inorganic Au* does not publish reports of studies conducted with domestic (kitchen) microwave ovens in which yields or selectivities observed using microwave irradiation are compared with results obtained using conventional heating.

For light-promoted reactions, report the light source: type of lamp along with manufacturer and model or type of lights, wavelength of peak intensity or broadband source, and available information about the spectral distribution and intensity; the identity and quantity or concentration of any photocatalyst or sensitizer; the material of the irradiation vessel if other than borosilicate glass; the distance from the light source to the irradiation vessel; and the use of any filters.

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. This acknowledgement is especially important in cases of "dual use" potential when the reported work could be directly misapplied by others to pose a threat to public health and safety. *ACS Organic & Inorganic Au* 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.

Compound Characterization 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. Characterization data and experimental details must be included in either the manuscript or the Supporting Information. It must be emphasized that the following is only a general guideline and authors are encouraged to present as much data as possible to support their structure assignments. In some cases, a reviewer or Editor may require authors to submit additional data to satisfy themselves of the validity of a proposed formulation.

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.

If required data cannot be obtained (a compound is too insoluble to record a carbon NMR, or too unstable to obtain a good elemental analysis, etc.), the reason for the absence of the data should be noted in the Experimental Section to avoid having review held up by a journal office request for the missing data. All compound preparation procedures and characterization data should be included in the manuscript, but at the authors' discretion may appear in the Experimental Section or in the Supporting Information, so long as the information is accurate and complete. Please see the ACS Research Data Guidelines and *The ACS Style Guide* for information on how to report data. For compounds that have been prepared by more than one method, the description in the Experimental Section and the purity documentation (usually a proton NMR spectrum in the Supporting Information) should clearly identify which method provided the sample whose yield and purity are documented.

Characterization Data

Routine Compounds

Compounds in this category are those that have either literature precedents or are obtained by a logical synthesis in close to quantitative yield.

When the preparation of known compounds *by a new or modified method* is reported, it is only necessary to report the yields, cite the published characterization data, and document the purity, usually by inclusion of proton NMR spectra or chromatograms in the Supporting Information (see section on Purity below). It is not necessary to include detailed NMR, IR, and MS peak listings in either the Experimental Section or Supporting Information unless erroneous data in the literature are being corrected, or unless the data are being reported for the first time.

For known compounds synthesized *by published methods* as reactants, reagents, catalysts, or study materials for physical or biochemical investigations, the literature data that were compared with the measured spectroscopic and physical data to confirm the materials' identity should be cited. Detailed synthesis procedures and listings of characterization data should not be included for these compounds unless the literature procedure has been substantially modified, or new physical or spectroscopic data are being presented.

Because of potential misidentification of atoms, an X-ray diffraction structure alone will not typically be considered to provide sufficient characterization for these molecules. Diamagnetic compounds must also be characterized by NMR spectroscopy, preferably for at least two different nuclei. In addition, at least one other characterization technique must be used to support the proposed formulation. Preferably, this would be a technique that provides definitive identification of a key functional group or chromophore. For example, IR spectroscopy may be used to support the presence of carbonyl, acyl, dinitrogen, carbonyl, and hydride moieties.

Paramagnetic compounds of this category present a further complication if NMR spectroscopy does not furnish clear evidence for the proposed formulation (note that NMR spectroscopy of

paramagnetic complexes can be useful if sufficiently large sweep widths are used). In many cases, X-ray diffraction may provide the most unambiguous characterization of such complexes, but this will not suffice as the only means of characterization. In the absence of an X-ray structure determination, evidence for elemental constitution must be provided by elemental analysis (e.g., combustion analysis, microprobe analysis), or mass spectrometry. Magnetic moment and/or ESR spectroscopic data should also be given for paramagnetic compounds if it is considered that the spin state of the molecule is of special interest.

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. In select instances, a variety of definitive spectroscopic techniques may provide sufficient characterization (e.g., if many of the nuclei are NMR active), but in the majority of cases evidence for elemental constitution must be provided by either elemental analysis (e.g., combustion analysis, microprobe analysis), or mass spectrometry. 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.

Solid State Materials

Compounds in this category are those that have no existence in solution. These materials 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.

Compounds that have not been isolated

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

Combinatorial Libraries

For combinatorial libraries containing more than 20 new compounds, complete characterization data must be provided for at least 20 diverse members of each structural type. Full characterization is not required for new compounds prepared solely as derivatives for analytical purposes (for example, Mosher esters prepared for assigning absolute configuration).

Mixtures of regioisomers, geometric isomers, and diastereomers

Mixtures of regioisomers, geometric isomers, and diastereomers (but not usually enantiomers) are generally expected to be separated, and the components individually characterized. When the components cannot be successfully separated and the individual gravimetric yields determined, the combined yield and the mole fraction of each component should be reported in the Experimental Section, and the spectroscopic or chromatographic method by which the composition was determined should be identified.

Identity. Evidence for documenting the identity of new compounds should include both proton and carbon NMR data and either MS accurate mass (HRMS) or elemental analysis data. Where other types of physical and spectroscopic methods are useful or necessary for confirming structure assignments, it is appropriate to include a summary of the data in the Experimental Section, but except as noted below, these additional data types are not generally required for routine compound characterization in *ACS Organic & Inorganic Au*. Such data types include IR, UV-visible, low resolution MS, GCMS, LCMS, 2D NMR (except where peak assignments are reported), and X-ray crystallography.

NMR. Please see the ACS Research Data Guidelines for organic chemistry data for more information on data requirements.

For enantioenriched or isotopically labeled forms of compounds whose racemic or unlabeled forms are known (or are fully characterized in the same manuscript), listings of NMR chemical shift data are not required, but either copies of NMR spectra, chromatograms, or other data are needed to document the chemical purity.

One of the purposes of including copies of NMR spectra in the Supporting Information is to qualitatively demonstrate the purity of the materials obtained when the reported reaction, isolation, and purification methods are used. It is not acceptable to use peak-editing software or other means to suppress or obscure peaks arising from impurities (including byproducts, unconsumed reactants, and incompletely removed extraction, chromatography, or recrystallization solvents). Peak suppression may be used on the NMR solvent peak for samples run in protic solvents, but it is never necessary for samples run in deuterated solvents.

Submission of spectra is strongly recommended for all new and/or key compounds, following these guidelines:

- A caption should be included on the spectrum, noting the nucleus being measured, the solvent (formula preferred, e.g. C_6D_6 over benzene-d_6) and the field strength.
- A representation of the compound should be included on the spectrum—please use ChemDraw or a related program. The compound identifier used in the manuscript should be included.
- The largest peak in the ^{1}H NMR spectrum should normally arise from the compound, not the solvent.
- All peaks in the ^{1}H NMR spectrum should be integrated. Chemical shift values should be included.
- The solvent peak should be clearly labeled on the spectrum.
- All peaks should be visible on the spectrum. Insets are encouraged to show expanded regions. At minimum, the spectral window should be 0 ppm to 9 ppm for ^{1}H NMR and 0 ppm to 200 ppm for ^{13}C NMR.
- Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

Elemental Analysis and Accurate Mass Measurement. Please see the ACS Research Data Guidelines for organic chemistry data for more information on data requirements.

When the scope of a new or modified synthetic method is illustrated with multiple examples, the description of each reactant or product that is a new compound needs to include elemental analysis or HRMS data. For information on characterizing large combinatorial libraries, see separate section on Combinatorial Libraries.

In reporting compounds prepared by linear, branched, or convergent multistep sequences, the characterization of at least every third compound needs to include elemental analysis or HRMS data. A new compound that is a branching point, a convergence point, or the final new compound in a synthetic scheme, needs elemental analysis or HRMS data regardless of whether the precursor or successor compounds are fully characterized or previously reported. A new compound that lacks elemental analysis or HRMS data should not have its name bolded in the

Experimental Section; instead, it should be described as an intermediate in the synthesis of the next fully characterized, bold-titled compound.

When a diastereomer or regiosomer mixture cannot be separated into its components, it is usually expected that elemental analysis or HRMS data will be reported for the mixture. Elemental analysis or HMRS data are not required for enantioenriched versions of compounds characterized as racemates in the same article or in the literature, or for the second enantiomer when the synthesis and isolation of both enantiomers is reported. In these cases, the chemical and enantiomeric purities of each enantiomer will need to be documented. Such enantiomers should have “racemate known” or “opposite enantiomer known” entered on the Compound Characterization Checklist to avoid a Journal office request for elemental analysis or HRMS data. Elemental analysis or HRMS data are not required for isotope-labeled versions of compounds already known in their unlabeled form unless such data are needed to demonstrate the extent of the labeling. A HRMS measurement is more useful than elemental analysis data when a transformation causes only a small change in the atomic composition (for example, hydrogenation of a carbon–carbon bond in a large molecule).

Accurate mass measurements should be performed at a mass resolution sufficient to minimize interferences. The reported molecular formulas and Calcd values should include any added atoms (usually H or Na). The ionization method and mass analyzer type (for example, Q-TOF, magnetic sector, or ion trap) should be reported. The number of potential molecular formulas within a given mass range centered on a measured (Found) value increases rapidly with molecular mass. A Found value within 0.003 *m/z* unit of the Calcd value of a parent derived ion, together with other available data (including knowledge of the elements present in reactants and reagents) is usually adequate for supporting a molecular formula for compounds with molecular masses below 1000 amu. Higher accuracy may be needed for compounds of higher mass, and for compounds of uncertain synthetic or biosynthetic origin, such as isolated natural products and their derivatives.

A single-crystal X-ray diffraction structure is generally an acceptable alternative to elemental analysis or HRMS data for confirming the molecular formula.

Configurational Isomer Mixtures. The composition of enantioenriched isomer mixtures and diastereomer mixtures, determined from NMR, chromatographic, or other data, should be reported. Either mole fractions, or enantiomer or diastereomer ratios, are preferred over enantiomeric or diastereomeric excess values. Copies of the spectra or chromatograms should be included in the supporting information.

Experimental Electronic Circular Dichroism and Vibrational Circular Dichroism Spectra. Experimental conditions of ECD and VCD spectra such as concentration, solvent, and optical path length should be indicated. Spectral intensities should be reported in units of molar absorptivity (, M^{-1} cm^{-1}). The method of baseline correction (subtraction of solvent or racemate spectrum) must be noted. The spectra should always be presented together with the corresponding unpolarized absorption spectra (UV/vis and IR) shown at the same scale. See also the section on Computational Data.

Oxygen Balance. Oxygen balance parameter gives potential of a compound or an explosive towards oxidation. Please report the oxygen balance in the following format including the complete formula used for calculation:

- Oxygen balance (OB, %) for CaHbNcOd: OB=1600×(d-2a-b/2)/Mw, Mw= molecular weight (based on carbon dioxide).

Specific Optical Rotation. Please see the ACS Research Data Guidelines for organic chemistry data for more information on data requirements.

Physical State and Melting Point. Please see the ACS Research Data Guidelines for organic chemistry data for more information on data requirements.

The description of new compounds should include a statement of whether the isolated material is a crystalline solid, an amorphous solid, a gum, or a liquid. The color should be reported if it is not colorless or white. Authors are encouraged to report melting point ranges for recrystallized

samples of known compounds that were previously reported only in noncrystalline (and presumably less pure) form.

Infrared and Low-Resolution MS. Please see the ACS Research Data Guidelines for organic chemistry data for more information on data requirements.

Purity and Yield. *ACS Organic & Inorganic Au* requires that purity be documented compound-by-compound, with copies of spectra or chromatograms, elemental analysis, or quantitative NMR or chromatographic integration data. The yield of all compounds 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.

When primarily synthetic work is reported, *ACS Organic & Inorganic Au* does not require that a certain minimum level of purity be met for the reported compounds, but it does require that the purity level that has been attained be faithfully documented. When new or known synthesized compounds are the study materials for physical measurements or bioassays, a purity level of at least 95% needs to be documented. Evidence for documenting compound purity should include one or more of the following:

- A standard 1D proton NMR spectrum or proton decoupled carbon NMR spectrum showing at most trace peaks not attributable to the assigned structure. A copy of a spectrum with a signal to noise ratio sufficient to permit seeing peaks with 5% of the intensity of the strongest peak should be included in the supporting information. The normal full range of chemical shifts should be displayed (usually 0–10 ppm for proton; 0–200 ppm for carbon). For *new* compounds, copies of both proton and carbon NMR spectra are required.
- Combustion elemental analytical values for carbon and hydrogen (and nitrogen, if present) agreeing with calculated values within 0.4%.
- Quantitative NMR data using an internal standard and based on peak area ratios determined under conditions that assure complete relaxation.
- Quantitative gas chromatographic analytical data for distilled or vacuum-transferred samples, or quantitative HPLC analytical data for materials isolated by column chromatography or separation from a solid support. The stationary phase, solvent (HPLC), detector type, and percentage of total chromatogram integration represented by the product peak should be reported. Alternatively, a copy of the chromatogram may be included in the supporting information.
- Electrophoretic analytical data obtained under conditions that permit observing impurities present at the 5% level.
- For *known* solid compounds, a narrow melting point range that is in close agreement with a cited literature value.

The type of evidence appropriate for demonstrating a compound's purity will depend on the method of preparation, the compound's air and thermal stability, structure complexity, the nature of likely impurities, and the amount of sample available. A narrow melting point range is not sufficient by itself to document the purity of a new compound. MS accurate mass (HRMS) data may be used to support a molecular formula assignment but cannot serve to document compound purity.

Biomacromolecules. The structures of biomacromolecules may be established by providing evidence about sequence and mass. Sequences may be inferred from the experimental order of amino acid, saccharide, or nucleotide coupling, from known sequences of templates in enzyme-mediated syntheses, or through standard sequencing techniques. Typically, a sequence will be accompanied by MS data to establish the molecular mass. A copy of a chromatogram, electropherogram, or blot should be placed in the supporting information to document the homogeneity.

Structural and Chemical Shift Data for Proteins and Nucleic Acids. Any set of atomic coordinates referred to in the manuscript, including 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 whenever appropriate. (Theoretical model depositions are no longer accepted for inclusion in the PDB archive.) If the coordinate files are not deposited in the PDB, or if the PDB files are on hold until publication, then the coordinate files must be included in the Supporting Information submitted concurrently with the manuscript. Requirements are similar for structures of nucleic acids, which should be deposited with the Nucleic Acid Database. A manuscript that does not provide coordinates at the time of submission will not be sent out for review. 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. If a file name has not yet been obtained upon acceptance of a manuscript, it must be added in proof. Atomic coordinates and structure factors for all structures mentioned must be available immediately upon publication of the article, either directly in the Supporting Information or as a data bank deposition. Similar requirements also apply to any chemical shifts referred to in the manuscript, whether they are only for assignment of resonances or used for any form of structure calculation. Those chemical shifts must be available to the reviewer at time of submission, either as an available entry in the Biological Magnetic Resonance Data Bank or included directly as Supporting Information.

Spectra. Reproductions of spectra will be published in the results and discussion section only when concise numerical summaries are inadequate for the discussion. Articles with a focus on interpretation of spectra, and those in which band shape or fine structure needs to be illustrated, may qualify for this exception. When presentation of spectra is essential, only the pertinent sections, prepared as figures, should be included. Spectra used as adjuncts to the characterization of compounds should be included in the Supporting Information.

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 is demonstrated.

Kinetic and Equilibrium Data. For publication in the *ACS Organic & Inorganic Au*, 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 STRENDA (Standards for Reporting Enzymology Data) Commission of the Beilstein Institut (http://www.beilstein-institut.de/en/projects/strenda/guidelines) for an example of detailed guidelines.

Nuclear Magnetic Resonance Pulse Sequences. For manuscripts that present new NMR pulse sequences, authors are requested to supply as “Supporting Information for Publication” a file that includes the original working pulse sequence information required to record data. This will typically include the pulse sequence code, parameter set, and other associated files, such as tables of gradient or pulse shapes.

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 where 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 Experimental Section. Tables of atom coordinates and thermal parameters will not be printed.

Supporting Information. See ACS Research Data Guidelines on organic chemistry data for complete details. Deposition of CIF files in the Cambridge Crystallographic Data Centre (CCDC) does not eliminate the *ACS Organic & Inorganic Au* requirement to submit the CIF file(s) as Supporting Information.

Authors are requested to combine multiple CIFs for a given manuscript into a single file. The individual structures in the combined file are to be separated from each other by the sequence #===END at the beginning of a new line. *ACS Organic & Inorganic Au* requires authors to run the CheckCIF program for each crystallographic structure and to correct any syntax errors in the CIF file prior to submission. Authors should consult the CIF Submission Instructions listed below during manuscript preparation.

Structure factors (except for proteins and nucleic acids) should not be submitted as Supporting Information. However, one printed table of structure factors should be retained in case it is requested by the Editor for review purposes only.

Powder Diffraction Data. The presentation of X-ray powder diffraction data for new materials or for materials previously uncharacterized by this technique is encouraged. 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 lines. Where resolution into $_1$-$_2$ doublets occurs, the identification of the *d* spacing for each line as d_1, d_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.

Magnetic Measurements. Fits of magnetic data [*(T)*, *-1(T)*, *T(T)*, *(T)*, *M(H)*, etc.] to an analytical expression must include both the Hamiltonian from which the analytical expression is derived and the final analytical expression and fitting parameters. When the value of an exchange coupling constant, *J*, is given in the abstract, the form of the Hamiltonian must also be included. The expressions may be included in the manuscript or, if long and complex, as Supporting Information; if the latter method is used, it should be noted in the Supporting Information paragraph at the end of the manuscript. In addition, how the sample was measured (in a gelatin capsule, Teflon capsule, etc.) and the diamagnetic correction for the sample holder, as well as the diamagnetic correction for the material, must be provided and the manner in which it was calculated (Pascal's constants) or measured must be stated.

Computations. See ACS Research Data Guidelines on organic chemistry data for complete details.

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 and Footnotes. 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. 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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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.

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Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through ACS Publishing Center, 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

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

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- there is evidence that the findings are unreliable but the authors’ institution will not investigate

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- 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.

Appendix 1: PREPARING FOR SUBMISSION

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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 communication or letter. Statement examples can be found in the Safety Statement Style Sheet and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* is freely available here.

Conflict of Interest Disclosure

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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.

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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.
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 Graphical Abstract service.

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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