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JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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Important Manuscript Submission Requirements and Notices

- When a manuscript is submitted to *JACS*, Editors must make an initial editorial judgment regarding its suitability for the journal's audience. A significant number of submissions are returned without sending them on for further processing.
- Titles of manuscripts may not contain the words "First" or "Novel" nor any part number or series number.
- Acronyms and abbreviations are not permitted in manuscript titles, unless they are broadly familiar to readers in all disciplines of chemistry.
- Title of manuscript, list of authors, and order of authors must be the same on all pieces of the submission.
- All authors must be listed on the submission page with current contact information and a direct/valid e-mail address for each.
- Communications and Articles must contain both an Abstract and a Table of Contents (TOC) graphic in the manuscript document file.
- A Communication must convey the scientific findings concisely in abstract, main text, and graphical elements **not exceeding 2200 words**.
- All sections of an Article must be properly labeled (Introduction, Discussion, Experimental Section, Conclusions, etc.).
- Turn "track changes" off before submitting files; upload annotated files as Supporting Information for Review Only.
- 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).
- All pages of the PDF Supporting Information should be numbered consecutively.
- Supporting Information may not be included in the manuscript document, but must be uploaded separately as Supporting Information for Publication or Supporting Information for Review Only.
- Simple equal authorship statements are allowed; itemization of individual author contributions or partial authorship is not permitted.
- Use of excessive self-citations is not permitted.
- Disclaimers are not allowed in *JACS* manuscripts or in the Supporting Information.
- Appendices may appear only in the Supporting Information, not in the manuscript.
- Trademarked items (company or institutional logos, images, and products) and images downloaded from the Web are not permitted, and all graphics are subject to approval by the Editor.
- Dedications may appear only in the Acknowledgment section and are subject to approval by the Editor.
- The receipt date will be recorded as the date the complete manuscript is received by the Editor's office. Manuscripts that are ready to be reviewed when first submitted will receive

priority for initial processing and assignment to an Associate Editor.
- The publication date will be recorded as the date the paper first appears online as an ACS Publications product—the earlier of “Articles ASAP” or issue publication date.
- Failure to adhere to one or more of the ACS Ethical Guidelines to Publication of Chemical Research will result in disciplinary action.

Scope of the Journal

The *Journal of the American Chemical Society* is published weekly and is devoted to the publication of fundamental research papers in all fields of chemistry. Articles, Communications, Perspectives, and Spotlights are published. “Notes” and “Comments” on earlier work are not considered or published. More information can be found here.

Manuscript Types

Articles most appropriate for publication in *JACS* are those that deal with some phase of “pure” chemistry as distinguished from “applied” chemistry, yet not all manuscripts that describe well-executed work can be accepted. Articles of high scientific quality, originality, significance, and conceptual novelty that are of interest to the wide and diverse contemporary readership of *JACS* will be given priority for publication. Articles on methodology should include one or more applications of widespread interest and, unless significant new advances are announced, will be declined with the recommendation for Manuscript Transfer to specialized journals. Papers that draw conclusions from the treatment of existing data must also include significant new data and make new experimental or theoretical predictions of broad interest. Articles which mainly expand findings that were previously published as Communications in *JACS* or elsewhere and which only incorporate experimental data, without greatly expanded scope and without providing new insights or conceptual breakthroughs, will be declined. Articles that are mainly routine extensions of previously published related work will also be declined with the recommendation 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).

Communications are restricted to reports of unusual urgency, timeliness, significance, and broad interest. A brief statement explaining how the manuscript meets the criteria of urgency and significance should be included in the author’s cover letter. It is desirable that the principal conclusions be stated in the opening sentences of the manuscript. Communications must conform to the length guidelines described in the ‘Preparation of Manuscripts’ section. The submission of multiple Communications on the same or closely related topics within a short period of time is not an acceptable means of publishing a body of work that is too large for a single Communication. Such work should be described in the format of an Article. The major concepts must not have appeared previously as a report or publication. If a previous Communication by the same author(s) has already appeared and the present manuscript describes a technical improvement or increase in the scope of the work, it will not be accepted in the absence of a novel conceptual advance.

A Communication must convey the scientific findings concisely in abstract, main text, and graphical elements as determined by word count not exceeding 2200 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. 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 Communication can be included as Supporting Information.

The current Communications templates (Microsoft Word 2011 for Macintosh and Microsoft Word 2010 for Windows) remain available for submission and will facilitate the review process; however, word count is the defining limit for a *JACS* Communication. Authors need not fit the manuscript to four strict pages by the template measure. 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. Communications exceeding the word count limit must be shortened before acceptance. Sample Communication in new template

Perspectives are personal reviews of a field or area, 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. The *JACS* 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. 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 topic. Perspectives should be no more than 9,000 words, including the abstract, main text, and figure captions.

ACS Publishing Center

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

- Mastering the Art of Scientific Publication, which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on how to prepare and submit a manuscript to ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, including details on selecting the applicable Journal Publishing Agreement.
- Sharing your research with the public through the ACS Publications open access program.
- ACS Reviewer Lab, a free online course covering best practices for peer review and related ethical considerations.

Manuscript Preparation

Submit with Fast Format

All ACS journals and partner journals have simplified their formatting requirements in favor of a

streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers here.

Manuscripts submitted for initial consideration must adhere to these standards:

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

Document Templates and Format

The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text.

- Microsoft Word 2011 for Macintosh
- Microsoft Word 2010 for Windows | README file

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

Acceptable Software, File Designations, and TeX/LaTeX

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

Cover Letter

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

The letter must provide the corresponding author’s name, postal and e-mail addresses, and telephone and fax numbers. 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 coauthors of the paper and for obtaining the coauthors’ assent to any substantial changes of content or interpretation made during revision. The cover letter may suggest the name of an appropriate *JACS* Associate Editor. However, manuscript assignment to an Associate Editor is ultimately at the discretion of the Editor. Authors must suggest a minimum of six to eight persons competent to review their manuscript. The selection of appropriate reviewers is the prerogative of the Associate Editor handling the manuscript.

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 use of a preprint server in the cover letter and include a link to the preprint, and as appropriate, state how the manuscript has been adjusted/updated between deposition and submission.

Manuscript Text Components

Title. The title should accurately, clearly, and concisely reflect the emphasis and content of the paper. Series or part numbers may not be used, nor may the words “Novel” or “First” appear in the title. Acronyms and abbreviations are not permitted in manuscript titles, unless they are broadly familiar to readers in all disciplines of chemistry.

Author List. Include as coauthors all those who have made substantial contributions to the work. Use first names, initials, and surnames (e.g., John R. Smith). Do not use only initials with surnames (e.g., J. R. Smith), because this causes indexing and retrieval difficulties and interferes with unique identification of an author. Deceased persons who meet the criteria for inclusion as coauthors should be so 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 author 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 coauthors must be provided on the Authors & Institutes page upon submission of the manuscript in the ACS Paragon Plus Environment.

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.

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, that address should be given in an Author Information note.

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 manuscripts (Communications and Articles) must contain an abstract, which should summarize the reason for the work, the most significant results, and the conclusions. The abstract should not exceed about 250 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.

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 paper, 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 (Communications). Section headings (Introduction, Experimental Section, Conclusion, etc.) should not be used in a Communication.

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 Section of the full article or the main text of a Communication.

Disclaimers. Disclaimers are not allowed in *JACS* manuscripts or in the Supporting Information.

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 Addresses note.

Simple equal authorship statements are allowed and may be presented in an Author Contribution note. However, itemization of individual author contributions or partial authorship is not permitted in any part of the manuscript or Supporting Information.

Associated Content. If the manuscript is accompanied by one or more Supporting Information files for publication, a brief description of each file is required. The descriptions should be placed at the end of the manuscript, before the list of references. ACS will add a sentence directing interested readers to the Supporting Information on the ACS Publications website via the paper's DOI.

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 on publisher Web sites. Because of this electronic linking, and to aid scientific research, *it is crucial that authors verify the accuracy of all reference citations and footnotes.*

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. Literature references and short explanatory footnotes must be

numbered with Arabic numerals in the order of their first citation in the text and the corresponding numbers placed at the appropriate locations in the text as superscripted numerals.

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. Supplementary references may be placed in Supporting Information.

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.

Authors should consult *The ACS Style Guide*, 3rd ed.; American Chemical Society: Washington, DC, 2006, for the appropriate style to use in citations of journal papers, 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.

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

any other materials necessary to reproduce or replicate the results.

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

Data Requirements

Characterization of New Substances. Adequate evidence to firmly establish both identity and purity should be provided. Recommended criteria vary according to substance categories. A summary of the detailed criteria may be found below.

Guidelines for Characterization of Organometallic and Inorganic Compounds

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 paper 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.

Characterization Data

(a) 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. 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 especial interest.

(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. In select instances, a variety of definitive spectroscopic techniques may provide sufficient characterization (for example, 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.

(c) Solid State Materials

Compounds in this category are those that have no existence in solution. While X-ray diffraction may provide the most unambiguous characterization of such compounds, evidence for elemental constitution and homogeneity needs to be presented. Atom ratios as determined by, for example, microprobe analysis of selected elements may be sufficient for this purpose

(d) 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 a paper be published in which none of the new compounds reported has been isolated and fully characterized.

Purity and Yield

The yield and purity 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.

Guidelines for Characterization of Organic Compounds

Sample Quality

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

Molecular Weight

Evidence of molecular weight should be provided, especially if elemental analysis was 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.

Miscellaneous

Numerical listings of characteristic spectroscopic data should be included to support assigned structures, changes in functionality, unusual chromophores, properties, 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 []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.

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.

Spectra. Reproductions of spectra, or the relevant segments thereof, will be published only if concise numerical summaries are inadequate for the purposes of the paper. Papers dealing primarily with interpretation of spectra and those in which band shape or fine structure needs to be illustrated may be published with such spectra included. Spectra will not be published merely as adjuncts to the characterization of compounds, however. See 'Supporting Information' below. Routine infrared, electronic, NMR, and mass spectra of new compounds should be numerically summarized, as appropriate, in the Experimental Section of an Article or in the Supporting Information of a Communication.

Kinetic and Equilibrium Data. For publication in the *Journal of the American Chemical Society*, 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.

Reporting and Stewardship of NMR Data. New guidelines recommend a standard baseline for the submission of NMR data to ACS journals. They are intended to promote accuracy and consistency. The guidelines are divided into three sections: NMR text, which outlines the preferred format for NMR data included in the Experimental Section; NMR spectra, which outlines the preferred format for inclusion of hard copies of spectra in the Supporting Information; and primary NMR data files, which outlines the procedure for submitting FID files, acquisition data, and processing parameters to include in the Supporting Information. Authors are strongly encouraged to provide all three sets of data for all new and/or key compounds described in a manuscript submission.

In the Experimental Section, the compound must be clearly identified, for example in a header at the beginning of the synthetic procedure or the summary of spectroscopic data. List the nucleus being measured, any nucleus being broad-band decoupled, the solvent used (formula preferred, e.g. C_6D_6 over benzene-d_6), the standard used, and the field strength. Field strength should be noted for each spectrum, not as a comment in the general Experimental Section. The standard(s) may be specified in the general Experimental Section; as an example, ^{1}H NMR data recorded in C_6D_6 listed as "residual internal C_6D_5H (7.15)". Indicate solvent or peak suppression protocols used in collecting data. List the probe temperature when it is accurately known; ambient probe temperature is otherwise understood. Give ^{1}H NMR chemical shifts to two digits after the decimal point. Include the number of protons represented by the signal, peak multiplicity, and coupling constants as needed (*J* italicized, reported with up to one digit after the decimal). The number of bonds through which the coupling is operative, ^xJ, may be specified by the author if known with a

high degree of certainty. Accepted abbreviations for multiplicities and descriptors are s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet (denotes complex pattern), dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, and br = broad signal.

Chemical shifts should be listed consistently in a single article, starting either from downfield to upfield or vice-versa. Assign peak identities under the following circumstances: non-decoupled or equivalent spectra have been collected (^{13}C, ^{31}P, etc.); 2-D experiments have been performed; or unambiguous assignment is possible without additional experiments, such as in the case of an organometallic metal-hydride ^{1}H signal, PF_6 vs $MPPh_3$ ^{31}P signal, etc. Give ^{13}C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks. Include peak multiplicities for ^{1}H-coupled ^{13}C NMR spectra or for signals in ^{1}H-decoupled spectra that are coupled to other magnetically active nuclei. A ^{13}C NMR signal will be considered a singlet if the multiplicity is not assigned. Only rarely is a true multiplet observed in a $^{13}C\{^{1}H\}$ NMR spectrum. However, a certain region may contain a group of unresolved peaks or signals. Mention of unobserved resonances is encouraged.

Submission of spectra (.doc, .docx, .txt, .pdf, .tif) 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 1 ppm to 9 ppm for ^{1}H NMR and 10 ppm to 180 ppm for ^{13}C NMR.
- Font should be clear and large enough to read (minimum of 10 point). Horizontal orientation is preferred for spectra.

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is encouraged for all new and/or key compounds. When submitting these files, please consider the following guidelines:

- One folder should be created for each compound. The folder should be named clearly, using the compound name (if available) and compound identifier, as referenced in the Experimental Section or Supporting Information. Include the FID files, acquisition data, and processing parameters for each experiment.
- Name each spectrum according to the type of nucleus measured. ^{1}H, ^{13}C, DEPT, COSY, etc. NMR files should be compressed into zip files—please use multiple zip files if necessary. Files must be submitted in their native format. In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e., 300 MHz ^{1}H or 50 MHz ^{13}C). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

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.

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 paper, it must be added in proof. Atomic coordinates and structure factors for all structures mentioned must be available immediately upon publication of the paper, either directly in the Supporting Information or as a data bank deposition. Similar requirements also apply to any chemical shifts referred to in the paper, 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.

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.

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.

CIF Submission Instructions:

All Crystallographic Information Files (CIFs), structure factor tables, and CheckCIF reports must be submitted to the Cambridge Crystallographic Data Centre (CCDC) **prior to manuscript submission**. See Requirements for Depositing X-Ray Crystallographic Data [PDF] for complete details on submission of CIFs and a list of file types accommodated by CCDC.

- Before being submitted to CCDC, CIFs should be checked using the free checkCIF data-validation utility on the CIF Validation site.
- Any reported syntax errors should be corrected. Authors are required to correct/defend/or respond to any A-level alerts. Comments may be inserted into the CIF file using a Validation Response Form or uploaded as a separate document as Supporting Information for Review Only.
- checkCIF output files (combined into one PDF file) should be uploaded at submission as Supporting Information for Review Only.
- Any subsequent revisions to the CIFs or structure factor tables should be deposited directly with the CCDC before resubmitting the manuscript in ACS Paragon Plus.

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

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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.

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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.

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.

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

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

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