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Intramolecular Hydroamination/Cyclization of Aminoallenes Catalyzed by Organolanthanide Complexes. Scope and Mechanistic Aspects

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New in 2015:

1. Templates with embedded graphics must be used for all submissions.
2. The preferred length of Communications is two journal pages.
3. No new submissions for Notes will be considered.

1 Scope and Editorial Policy

1.1 Scope of the Journal

Organometallics publishes original contributions on fundamental studies of all aspects of organometallic chemistry. Among the areas included are the following: **SYNTHESES** of organometallic compounds; **STRUCTURE** and **BONDING**, experimental and theoretical studies; **CHEMICAL REACTIVITY** and **REACTION MECHANISMS** of the metal–carbon bond as well as of other organic and inorganic functionalities present in the molecule; **APPLICATIONS**, organometallic reagents in organic, inorganic, and polymer synthesis; catalytic processes in which an organometallic compound is the precatalyst or catalyst or in which

organometallic species are intermediates; organometallic compounds in materials science, green chemistry, energy science, solid-state chemistry; bioorganometallic and environmental organometallic chemistry.

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

1.2 Restrictions on Scope and Content

1.2.1 Prior Publication. Manuscripts submitted to *Organometallics* must, except for reviews, be based upon original research by the authors. The manuscript may be precluded from consideration for publication if it deals with information that has been made publicly available in print or electronic format. Such disclosure includes posting of conference presentations, posters, and preprints on Web sites. All such print or electronic materials, with the exception of short abstracts, must be itemized in the cover letter.

An exception to these disclosure restrictions is the final version of a thesis filed as a publicly stated requirement for a degree and posted on the official Web site of the degree-granting institution.

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

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

1.2.3 Other. Excessive fragmentation in the publication of research in a given area is a disservice to the community and can be grounds for rejection.

1.3 Types of Manuscripts Published

Articles (full papers), communications, and reviews are regularly published.

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

1.3.2 Communications are meant to provide rapid, preliminary publication of new developments in organometallic chemistry that will be of particular significance and interest to readers and promise to influence the future work and thinking of other chemists. The preferred length for Communications is two journal pages; in special circumstances and with approval of the Editor in Chief, Communications of three or

four pages may be considered.

1.3.3 Reviews are normally prepared following correspondence with the Editor-in-Chief. They may be published in several formats, including but not limited to personal accounts, comprehensive reviews, and historical overviews. Authors should make the type and scope of the review clear to readers in the opening paragraphs. For comprehensive reviews, all contributors to the subject are to be treated on an equal footing when selecting material for an in-depth discussion. This is relaxed for personal accounts, but authors are encouraged to attribute credit to prior researchers and acknowledge contemporary efforts by others. Reviews do not contain significant amounts of new experimental data or data that have not been peer reviewed.

1.3.4 Additions and Corrections. If errors or omissions of consequence are detected in the published paper, the authors should upload a correction using the Paragon Plus Web site. After review, these will be published in the "Additions and Corrections" section. Additions and Corrections may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the ACS Paragon Plus environment by the corresponding author for publication in the "Addition/Correction" section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction, or provide evidence that such approval has been solicited. The Addition and Correction should include the original article title and author list, citation including DOI, and details of the correction. For proper formatting, see examples in a current issue of the Journal.

1.3.5 Retractions. Articles may be retracted for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. Retractions may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of Retraction will be published containing information about the original article title, author list, and the reason for the Retraction. Retracted articles will be accompanied by the related Retraction notice and will be marked as "Retracted". The originally published article will remain on the web except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information see: <http://publicationethics.org/>."

Special notices concerning newly encountered, unexpected examples of the pyrophoric, explosive, or toxic nature of organometallic compounds or of special hazards encountered in organometallic reactions will also be considered for publication. Authors who encounter such safety hazards are encouraged to report them without delay.

2 Ethical Issues

All authors of any manuscript are expected to review the "Ethical Guidelines to Publication of Chemical Research" (<http://pubs.acs.org/page/policy/ethics/index.html>), which outlines the ethical obligations of editors of scientific journals, of authors who submit manuscripts to such journals, and of reviewers of these manuscripts.

The entire community is encouraged to read these guidelines with care. They should be kept in mind by authors when they are preparing any manuscript for submission, and by the reviewers to whom these manuscripts are sent.

If an author has good reason to believe that one of the editors or reviewers has not met one or more of these ethical obligations, a formal appeal with the Editor in Chief of this journal may be filed. Any evidence relating to such a case will be considered with care, and as quickly as possible, by the Editor in Chief, in some cases in

collaboration with one or more of the Associate Editors, with the objective of adjudicating the matter in question.

A statement describing any financial conflicts of interest or lack thereof is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest (please see the ethical guidelines; advising is also available at support@services.acs.org). The statement will be published in the final article. If no conflict of interest is declared, the following statement will be published: "The authors declare no competing financial interest."

3 General: Manuscript Submission through Publication

3.1 Manuscript Submission and Evaluation

Manuscripts should be submitted on the American Chemical Society (ACS) Paragon Plus Web site at <http://acs.manuscriptcentral.com/acs>. In the course of this guided procedure, authors are required to:

- (a) provide the names of all authors and their institutional addresses (these must match those given on the cover page of the manuscript);
- (b) provide the names of potential critical reviewers (special relationships to any of the recommended reviewers, and the basis for suggesting that any individual not be used as a reviewer ("non-preferred reviewer"), should be explained in the cover letter);
- (c) indicate whether the manuscript has been previously considered by another journal;
- (d) confirm that the manuscript has been prepared in accordance with the ACS Ethical Guidelines to Publication of Chemical Research.

Requests for evaluation by specific Associate Editors are welcome but cannot always be honored due to workload, availability, and expertise considerations.

For manuscripts that have been previously declined by another journal, copies of all earlier correspondence and reviewer reports concerning the manuscript should be uploaded as well (as an appendix to the cover letter, or as "supporting information for review only"). The authors must describe the revisions that have been made in response to previous reviewer reports and/or Editor input. This should be in the form of a text document in which each reviewer/Editor suggestion is followed by the action taken (color or bold/italics coding recommended).

Cover letters should be addressed to the Editor in Chief, unless invited by a Guest or Associate Editor for a special issue. For manuscripts without a prior history, authors are encouraged to simply paste their cover letter into the text box provided in Paragon Plus and forego attaching a formal letterhead document.

A properly completed and signed Journal Publishing Agreement must be submitted for each manuscript. ACS Paragon Plus provides an electronic version of the Agreement that will be available on the **My Authoring Activity** tab of the Corresponding Author's Home page once the manuscript has been assigned to an Editor. A PDF version of the Agreement is also available, but **Authors are strongly encouraged to use the electronic Journal Publishing Agreement**. If the PDF version is used, **all pages of the signed PDF Agreement must be submitted**. If the Corresponding Author cannot or should not complete either the electronic or PDF version for any reason, another Author should complete and sign the PDF version of the form. Forms and complete instructions are available at <http://pubs.acs.org/page/copyright/journals/index.html>.

Authors may want to have their manuscripts edited professionally before submission to improve clarity. The ACS ChemWorx English Editing Service can assist you in improving and polishing the language in your manuscript.

You can learn more about the services offered, at <http://es.acschemworx.acs.org>.

During manuscript submission, the submitting author is asked to select funding sources from the list of agencies included in the FundRef registry: <http://www.crossref.org/fundref/>.

Requirements regarding the submission of revised manuscripts (cover letter, time limits, etc.) are communicated through the Paragon Plus system when the reviewer reports are returned.

3.2 Proofs and Publication

The corresponding author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via a secure Web site. Authors will access the secure site through ACS ChemWorx and will need an ACS ID. To obtain an ACS ID or to reset your password, go to <http://www.acschemworx.org> or contact support@services.acs.org.

Routine rephrasing of sentences or additions are not permitted at the page proof stage. Alterations should be restricted to serious changes in interpretation or corrections of data. Extensive or important changes on page proofs, including changes to the title or list of authors, are subject to Editorial review.

All manuscripts accepted for publication in ACS Journals will be posted in the Web edition of the journal as soon as possible after the author has corrected the proofs. This can occur within hours of receipt of proof corrections and be well in advance of the issue. Authors must plan their intellectual and patent activities related to a manuscript with this turnaround time in mind. The actual date on which the manuscript is posted on the Web is recorded in a separate line at the bottom of the first page in the PDF version of the paper.

All correspondence concerning *accepted* manuscripts, e.g., inquiries about status, publication date, proofs, etc. and requests to make changes or modifications, should be communicated to the email address acsproof@acs.org with the manuscript number in the subject line, or contact Journal Publications, Publications Division, American Chemical Society, P.O. Box 3330, Columbus, OH 43210 ((614) 447-3600, ext. 3171, or (614) 447-3665); FAX (614) 447-3745.

3.3 ACS Policies for E-prints and Reprints

Under the ACS Articles on Request policy, the Society will provide (free of charge) to all contributing authors a unique URL within the ACS website that they may e-mail to colleagues or post on external websites. These author-directed links are designed to facilitate distribution of an author's published work to interested colleagues in lieu of direct distribution of the PDF file by the author. The ACS Articles on Request policy allows 50 downloads within the first year after publication and unlimited access via the same author-directed links 12 months after publication.

3.3.1. ACS AuthorChoice Open Access

ACS AuthorChoice options establish fee-based mechanisms for authors or their research funding agencies to sponsor the open availability of final published articles on the Web. *ACS AuthorChoice* offers authors a wide range of open access license options, such as Creative Commons licenses and provisions for immediate or 12-month embargoed open access, and includes [ACS Certified Deposit](#). Authors will find useful information about compliance with open access policies available [here](#) and FAQs [here](#). Corresponding authors who published with ACS during 2014 may have access to *ACS Author Rewards*, a \$60M stimulus program ACS provided to help authors transition to new open access publishing models.

Authors must sign the Journals Publishing Agreement. Forms and complete instructions are available at <http://pubs.acs.org/page/copyright/journals/index.html>. After acceptance, authors will be presented with the opportunity to purchase an *ACS AuthorChoice* option, and authors who do so will be presented with the appropriate license at that time. For a review of all license options available, see <http://pubs.acs.org/page/4authors/authorchoice/options.html#optiona>. For questions or further assistance with

ACS AuthorChoice, please reach out to support@services.acs.org.

Upon receipt of the proof of their paper, authors will receive a link to a website where they may order author reprints. They may also call Cierant Corporation at (866) 305-0111 from 9AM to 5PM EST. Reprints will be shipped within two weeks after the issue publication date. Neither the Editors nor the Washington ACS Office keeps a supply of reprints; requests for single copies of papers should be addressed to the corresponding author of the paper concerned. Individual issues can be purchased on demand by clicking the Order Print Copy button on the issue page of the journal website.

4. Preparation of the Manuscript and Supporting Information

4.1 Special Author Resources

Authors are encouraged to consult the ACS Author and Reviewer Resource Center for a variety of helpful materials and guides; see <http://pubs.acs.org/page/4authors/submission/index.html>. Another useful document is entitled "10 Secrets for Successful Article Submissions": <http://pubs.acs.org/page/pr/successful-submissions.html>.

The ACS Style Guide (3rd ed., 2006, Oxford University Press, ISBN 0-8412-3999-1) provides a comprehensive summary of the manuscript preparation, review, and production processes.

4.2 Page Formatting and Templates

Templates are required for the preparation of all manuscripts (<http://pubs.acs.org/page/orgnd7/submission/authors.html>). All equations, tables, graphics must be embedded in context such that they facilitate the peer review process. The template is built with fonts and spacing that approximate composed page length. Authors submitting page limited manuscripts should not manipulate the template to fit copy.

4.3 Manuscript Organization

The sections of an Article are:

- Title
- Authors' names and institutional addresses
- Graphic for Table of Contents and Abstract
- Abstract
- Introduction
- Results
- Discussion (may be combined with Results)
- Conclusion
- Experimental Section
- Associated Content (including Supporting Information statement)
- Author Information
- Acknowledgments
- References and Footnotes
- Supporting Information (including any CIF files or computational files)

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

4.3.1 Title. The title should accurately, clearly, and concisely identify the subject and emphasis of the reported work. Words should be chosen carefully to reflect the content and to function as indexing terms. The use of manuscript titles to make claims of priority, originality, convenience, effectiveness, or value should be avoided. For example, the words "concise", "convenient", "efficient", "elegant", "expedient", "facile", "first", "new",

"novel", "practical", "simple", "unique", "unprecedented", and "versatile" should be used with restraint and careful consideration.

4.3.2 Authors' Names and Institutional Addresses. In general, the given name, middle initial or name (if any), and surname of each author should be given. The name(s) of the corresponding author(s) should be marked with an asterisk (*).

The names and addresses of the institution(s) where the work was performed should be listed in the following paragraph. All author/address data must match that uploaded into Paragon Plus (see 3.1). If the coauthors are not all at the same institution or department, the institutional affiliation of each author should be indicated by labeling the institution names, using the symbols †, ‡, §, and ||, which are placed as superscripts after the appropriate author names.

If any corresponding author is no longer at the institution where the work was performed, a footnote, marked with an asterisk (*) rather than a number, should give that author's current address. Address changes may similarly be indicated for other authors. The text for these footnotes is collected in the "Author Information" statement; see section 4.3.10 below.

4.3.2.1. ORCID

All authors are encouraged to register for an ORCID iD, a unique researcher identifier. With this standard identifier, you can create a profile of your research activities to distinguish yourself from other researchers with similar names, and make it easier for your colleagues to find your publications. Learn more at <http://www.orcid.org>

Authors and reviewers can add their ORCID iD to, or register for an ORCID iD from, their account in ACS Paragon Plus. Submitting authors have the option to provide existing ORCID iDs for coauthors during submission, but they cannot create new ORCID iDs for coauthors.

4.3.3 Graphic for Table of Contents and Abstract. A graphic is required that will appear both (1) in the table of contents (TOC) of the issue in which the manuscript is published and (2) in the published paper within the abstract box. The graphic should capture the reader's attention and, in conjunction with the manuscript title, should give a quick visual impression of the content of the paper.

The TOC graphic should not exactly duplicate a graphic appearing within the text of the manuscript. It may be up to 3.25 in. (8.5 cm) wide and 1.75 in. (4.75 cm) tall. Further guidelines with examples of good and poor graphics may be found on the web at http://pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf. The TOC graphic is best inserted between the institutional address and the abstract, where it will appear in print, but placement at the end of the manuscript is also accepted. The use of crystal structures, especially as dominant elements, is discouraged.

4.3.4 Abstract. Abstracts are required for Articles, Communications, and Reviews. Abstracts for Articles and Reviews should not exceed 300 words, and those for Communications should not exceed 200 words.

Abstracts should be *informative* (purpose of study, principal results, major conclusions) and *self-contained*. Abbreviations and numerical designations (e.g., compound numbers) must be defined. For brevity, the latter are not allowed unless the number is needed later in the abstract.

4.3.5 Introduction. The introduction should place the work in the appropriate context and clearly state the purpose and objectives. An extensive review of prior work is not appropriate, and documentation of the relevant background literature should be selective rather than exhaustive, particularly if reviews can be cited.

Articles may use the heading "Introduction"; however, the opening paragraphs of some manuscript types may serve a similar function, although they are not labeled "Introduction".

4.3.6 Results and Discussion Sections. The presentation of experimental details in the Results section should be kept to a minimum. Reiteration of information from tables, figures, or reaction schemes should be minimized.

A separate Results section and Discussion section can be advantageous. The experimental or computational data in a Results section should normally be as valid 10 years from now as they are today. The analyses and models developed, which may be time-dependent, particularly as new data become available or instrumental or computational methods develop, are then clearly localized in a Discussion section.

Certain types of routine results of lesser interest to general readers (spectra of routine monitored reactions, tabular data generated from computer programs, chromatograms establishing (enantiomeric) purities, graphs, etc.) are often best presented in "Supporting Information for Publication".

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

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

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

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

Special attention should be called to hazardous compounds or operations, and appropriate precautions should be described. Literature citations should be provided for compounds or classes of compounds claimed to be toxic. Unsubstantiated claims of toxicity are not permitted.

Section 5 ("Specialized Data and Information") should be consulted for guidance on reporting synthetic, characterization, spectroscopic, crystallographic, and computational data.

A "General Methods" paragraph may be provided to document protocols (such as purification methods and spectroscopic and chromatographic analyses) that are common to most of the individual procedures. It should be placed at the beginning of the experimental section. Alternatively, a reference to the General Methods paragraph in an earlier publication may be provided.

Sources of reactants, reagents, and solvents need not be identified except for (1) starting compounds that are unusual or not widely available and (2) materials for which the author has evidence that the source is critical to the outcome of an experiment. Experiments involving a catalyst, enzyme, or reagent that is neither commercially available nor prepared by a described or clearly cited nonproprietary method may not be reported.

4.3.9 Associated Content Statement. This section is used to alert the reader to all materials not contained in the main body of the manuscript. Most commonly this is Supporting Information. If the manuscript is accompanied by any supporting information for publication, a brief description is required in the manuscript. The appropriate format is:

Supporting Information. [concise list of types of data being furnished]

A similar statement should be supplied regarding any web enhanced objects (WEOs). These may be files that

include color figures (including 3D rotatable figures), animations, spectra, video, and sound. Descriptions of WEOs should be included in the appropriate places within the related graphic caption or text of the paper, noting the type of file and format. Example: "a text file of all computed molecule Cartesian coordinates in .xyz format for convenient visualization." Links to WEOs will appear in the Web HTML edition of the paper. Files suitable for this form of publication should be viewable with commonly available Internet plug-ins or helper applications, and additional specifications can be found here: <http://pubs.acs.org/page/4authors/submission/weo.html>.

4.3.10 Author Information Statement. The e-mail address(es) of the corresponding author(s) should be given after a subheading "Corresponding Author".

Address changes for any author can be indicated after a subheading "Present Addresses". These should be connected to footnotes given after the author's name in section 4.3.2.

Any deceased authors should also be designated with footnotes.

4.3.11 Financial Interests of Authors. All authors are required to indicate any financial interests that they hold that could be a possible origin of bias in the reported research, as described in section 2 (Ethical Issues). When submitting a manuscript to the Journal via ACS Paragon Plus, the submitting author is asked to identify the funding sources for the work presented in the manuscript. Identifying funding sources is optional during submission of an original manuscript. Funding source information is required when a revised manuscript is submission. For inquiries regarding conflict definitions and appropriate text under various circumstances, authors should consult the help desk at support@services.acs.org.

4.3.12 Author Photographs and Biographical Sketches. For all reviews and certain invited articles, a photograph and biographical sketch of the corresponding author are required. Photographs and biographical sketches of coauthors are optional. These are inserted into the manuscript at the end of the Author Information Statement after a subheading "Biography" or "Biographies". Photographs must be accompanied by appropriate copyright forms, which will be provided by the Editor's office, and uploaded as "supporting information for review only".

4.3.13 Acknowledgments. This section may be used to acknowledge discussions with other researchers, technical assistance, gifts of starting materials or reference samples, data from individuals who provided spectroscopic, analytical, crystallographic, or graphical services but who are not coauthors, and financial support.

Acknowledgments are not to be used for "vanity purposes", such as mentioning an institutional teaching award, an ACS Award, a medal of honor, or other prize that did not contribute to the support of the work described.

4.3.14 Dedications. Dedications associated with special issues are given in a separate section after the acknowledgements. Otherwise, dedications are given within the acknowledgements.

4.3.15 References. All references and footnotes must be combined into a single consecutively numbered list at the end of the manuscript text under the heading "References". They should be numbered with Arabic numerals in the order of their first citation in the text, and the corresponding citation numbers should be inserted at the appropriate locations in the text as superscripted numerals without parentheses or brackets.

Authors should be judicious in citing the literature; unnecessarily long lists of references and self-citations should be avoided, particularly if recent reviews are available. If a number of publications are relevant to a statement in the text, consider citing two or three of the most seminal ones, or only the most recent paper from several research groups. If appropriate, the author may add "and references cited therein" following a reference.

It is the professional and shared responsibility of every author to ensure that all citations are complete and accurate. Each reference should be checked to make certain that it features the (a) correct year, (b) correct volume, (c) correct page number, (d) correct author surname, (e) correct author initials. References must be provided in ACS format, and if inclusive page numbers are given, they must be in complete and not truncated form (e.g. 3210–3214, not 3210–14). Articles that have not been read by any of the authors (for example, taken

without personal review from another source) should not be cited.

When articles are cited that have been submitted for publication, or are in press but not yet available on the web, copies should be uploaded for the Editors and reviewers as "Supporting Information for Review Only". Citations of personal communications of unpublished results from other researchers are discouraged.

Authors should consult recent issues of ACS journals and Chapter 14 of *The ACS Style Guide* (3rd ed., 2006, Oxford University Press; see <http://pubs.acs.org/userimages/ContentEditor/1246030496632/chapter14.pdf>) for the appropriate formats to use in citations of journal papers, books, and other publications. The abbreviations for the most frequently cited journal titles may be found in *The ACS Style Guide* or on the Web at <http://www.cas.org/expertise/cascontent/caplus/corejournals.html>.

For patents, for journals not published in English, and for journals that are not easily obtainable by most readers, a *Chemical Abstracts* citation should also be given.

Digital object identifier (DOI) numbers are an accepted form of citation before and after an article appears in print. These are supplied by the ACS and most other publishers at submission or with the proofs. DOI numbers should be furnished for papers published online too recently to have publisher-assigned page numbers (Articles ASAP for ACS journals), and for reports published only online.

4.3.16 Supporting Information. All supporting information must be in a separate file from the main text, and uploaded separately. The first page must begin with the title of the manuscript, the author names, and their affiliations in the same format as the first page of the main text. It is recommended that pages, references, Figures, Tables, etc. be distinguished with the upper or lower case letter "S" or "s" (e.g., page S1 or s1, reference S1 or s1, Figure S1 or s1, Table S4 or s4).

4.3.16.1 Non-Crystallographic and Non-Computational Data. All data intended for publication via the web, except for the files discussed in section 4.3.14.2 below, must be uploaded as a single file entitled "**Supporting Information for Publication**". Other required materials noted above (e.g., manuscript history information, preprints of work referenced as "submitted", etc.) must be uploaded as a single file entitled "**Supporting Information for Review Only**".

For Articles, the bulk of the experimental section should be presented in the main text, as detailed in section 4.3.8.

4.3.16.2 Crystallographic Data. For manuscripts with crystal structures, the following are required: (a) a properly formatted and computer-readable CIF file, uploaded as "Supporting Information for Publication" and (b) the corresponding checkCIF file(s) (see <http://checkcif.iucr.org/>), uploaded as "Supporting Information for Review only".

CIF files must be denoted as such in the File Format menu when uploading (choose .cif; no other formats will be accepted). Authors are encouraged to include structure factors in all CIF files, paralleling the requirement instituted by *Acta Crystallographica* to facilitate the detection of fraudulent crystal structures.

Data for multiple crystal structures should be combined into one CIF file (see <http://pubs.acs.org/page/orgnd7/submission/cif.html>).

Additional requirements dealing with the quality standards expected for crystal structure determinations are provided in Section 5. Deposition of CIF data at the Cambridge Crystallographic Data Centre (CCDC) does not fulfill the ACS requirements for deposition of Supporting Information.

4.3.16.3 Cartesian Coordinates obtained from Computational Studies. For manuscripts with computations, Cartesian coordinates for all computed molecules, intermediates, transition states, etc. that are part of the work are to be uploaded as a separate file as specified in section 5.8. Coordinates for all computational structures must be concatenated into a single file (multiple files are not allowed).

The following statement should be included in the Supporting Information document (section 4.3.16.1): “The supplemental file *filename* contains the computed Cartesian coordinates of all of the molecules reported in this study. The file may be opened as a text file to read the coordinates, or opened directly by a molecular modeling program such as Mercury (version 3.3 or later, <http://www.ccdc.cam.ac.uk/pages/Home.aspx>) for visualization and analysis.

Additional requirements are provided in Section 5.8.

5 Specialized Data and Information

5.1 Nomenclature

It is the authors' responsibility to provide correct, informative, and unambiguous nomenclature that conforms with current usage. Systematic names similar to those employed by Chemical Abstracts Service (CAS) and the International Union of Pure and Applied Chemistry (IUPAC) are encouraged. However, rigid and consistent conformance to these recommendations is challenging with organometallic compounds. The nomenclature employed should at a minimum accurately give the stoichiometric and topological composition of a compound.

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

Chemical Abstracts nomenclature rules are described in Appendix IV of the *Chemical Abstracts Index Guide*. A list of ring systems, including names and numbering systems, is found in the *Ring Systems Handbook*, American Chemical Society, Columbus, OH, 1993, and its latest cumulative supplement. Current IUPAC nomenclature recommendations can be found on the Web at <http://www.acdlabs.com/iupac/nomenclature> and <http://www.chem.qmul.ac.uk/iupac>.

5.2 Abbreviations

A list of accepted abbreviations may be found in Appendix 10-2 of *The ACS Style Guide* (3rd ed., 2006, Oxford University Press). Appropriate formats for units are summarized in Chapter 11. Symbols for physical quantities should be italicized (for example, *c*, *E_a*, *J*, *m/z*, *t*_{1/2}).

5.3 Experimental Section: Syntheses

Each paragraph describing a synthesis experiment should begin with the name of the product (see section 5.1) and any structure number assigned to the compound in the Results section. Thereafter, the compound should be identified by its structure number. Use of standard abbreviations or unambiguous molecular formulas for reagents and solvents, and of structure numbers rather than chemical names to identify starting materials and intermediates, is encouraged.

Reactant and product quantities should be given in both weight and molar units. It should be unambiguous whether yields pertain to a crude product (specify purity if possible) or a purified product. If yields are determined chromatographically, details (standards, response factors, means of correlating the peak to a structure, etc.) should be provided.

5.4 Experimental Section: Compound Characterization

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

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

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

5.4.1 Purity. Authors are required to submit microanalytical data for all new compounds. Carbon and hydrogen analyses should be supplied; data for additional elements (nitrogen, phosphorus, chlorine, etc.) are encouraged.

Agreement of calculated and found values within 0.4% (e.g., 20.14% vs 20.54%) is considered acceptable. For deviations that are slightly greater, authors may include footnotes along the lines of "although these results are outside the range viewed as establishing analytical purity, they are provided to illustrate the best values obtained to date". Authors are not obliged to supply a correct microanalysis of a mixture of isomers, although these are often successful, thereby establishing a "pure mixture".

With oils and some classes of compounds, correct microanalyses can be difficult to obtain. In these cases, the authors can (for diamagnetic compounds) supply copies of NMR spectra (^1H and ^{13}C required; ^{31}P and other nuclei encouraged when relevant) that establish the absence of detectable contaminants in the Supporting Information. These should be formatted per the "NMR Guidelines for ACS Journals" (http://pubs.acs.org/paragonplus/submission/acs_nmr_guidelines.pdf).

Manuscripts may occasionally be considered in which there has been no effort to obtain microanalytical data, but for which the NMR spectra have been supplied as described in the preceding paragraph.

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

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

5.4.2 Identity. **5.4.2.1 Melting Points.** All homogeneous solid products (e.g., not mixtures of isomers) should be characterized by melting or decomposition points. The colors and morphologies of the products should also be noted.

5.4.2.2 NMR Spectroscopy. For all new diamagnetic substances, NMR data should be reported (^1H , ^{13}C , and relevant heteronuclei). This should include the field strength, the solvent, any nuclei being decoupled, and other parameters as detailed in the "NMR Guidelines for ACS Journals" (http://pubs.acs.org/paragonplus/submission/acs_nmr_guidelines.pdf). It is strongly recommended that spectra of new compounds be depicted in the supporting information, formatted as described in the NMR Guidelines. Any 2D methods used to aid in peak assignments should be described.

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

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

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

The checkCIF files of all structures should be free of serious alerts, in particular A-level alerts. When such alerts persist despite conscientious attempts to remove them, authors are required to provide explanatory comments. These are preferably supplied as text inserted at the end of the CIF file using the Validation Response Form (VRF) command. For further details, consult <http://journals.iucr.org/services/cif/checking/checkfaq.html>. When properly implemented, the comments inserted using the VRF command will appear in the checkCIF file as "Author Response" directly below the relevant alert. Alternatively, authors may directly insert explanatory text below the alert in the checkCIF file.

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

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

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

5.4.2.4.3 Structural Representations. Color may be used in representations of crystal structures. The following Web sites offer guidance on atom coloring conventions:

<http://jmol.sourceforge.net/jscolors>

http://en.wikipedia.org/wiki/CPK_coloring

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

5.5 Tables

Tables should be used only if they present information more effectively and more efficiently than running text. They should be prepared in accord with the guidelines in Chapter 16 of *The ACS Style Guide*.

5.6 Graphics

Graphics should be prepared in accord with the guidelines in Chapters 15 ("Figures") and 17 ("Chemical Structures") in *The ACS Style Guide*. Each graphic should be composed for publication in single column width (8.25 cm, preferred) or double column width (17.78 cm). The judicious use of color is allowed.

5.7 Reproducing Previously Published Graphics or Materials

Manuscripts incorporating graphics, tables, equations, etc. from an earlier copyrighted publication must be accompanied by a letter from the copyright holder granting permission to reproduce the material in question. The web sites of most publishers have pages or forms by which one can request permission. The letter of form granting permission should be uploaded as "Other files for Editors only". Permission is not needed when the material is from a paper by one of the authors published in an ACS journal.

The source of the reprinted material should be identified in the caption. Typical credit lines can be found in Chapter 15 of *The ACS Style Guide* (see Box 15-7).

5.8 Computational Reports

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

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

5.8.2 Details of the computations. Final optimized coordinates and keywords are to be provided. For DFT computations, the choice of functional must be justified, or the validation of the functional provided. The choice of basis sets must be explicitly discussed, including any deviation from standard basis sets. Convergence criteria, integration parameters, active space definition in multireference calculations, and, for open-shell systems, the way in which spin states are handled should be mentioned explicitly. The exact definition of any applied numerical or symmetry constraint should be indicated.

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

5.8.4 Cartesian Coordinates. As outlined in 4.3.16.3, Cartesian coordinates of all molecules, intermediates, transition states, etc. that are part of the manuscript must be uploaded in a single file that is formatted for convenient viewing with widely-available molecular modeling packages. The .xyz and .mol formats are accepted at this time. The .xyz format is the most basic and easily prepared from computational output.

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

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

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

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

The file name should have the extension “.xyz”. A simple example with three molecules is shown in Table 1 (below).

It is strongly recommended that authors view the structures in the file with a modeling program before uploading the file. The program **Mercury** (version 3.3 or later) is recommended for viewing and manipulating the multiple structures. The Cambridge Crystallographic Data Centre (CCDC) offers **Mercury** at no cost at <http://www.ccdc.cam.ac.uk/pages/Home.aspx>.

Include the phrase “a text file of all computed molecule Cartesian coordinates in a format for convenient visualization” in the Supporting Information statement (section 4.3.9).

Table 1. Example 3molecule.xyz file containing CO, CH₄, and H₂O created by text editing for CO and CH₄ and copy-and-pasting of coordinates from the output of a computation for H₂O (notice the variable spacing and variable number formats allowed in the free-field format)

2
carbon monoxide, electronic energy = -0.57115848 a.u.
C 0 0 0
O 0 0 1.1512345678

5
Methane, electronic energy = -0.70771290 a.u.
C 0 0 0
H .5 .5 .5
H -.5 -.5 .5
H .5 -.5 -.5
h -.5 .5 -.5

3
Water, electronic energy = -0.54307351 a.u.
H -0.768340934 0.000000000 -0.106744877
O 0.000000000 0.000000000 0.513451800
H 0.768340934 0.000000000 -0.106744877
