Unique Reaction Path in Heterogeneous Catalysis: The Concerted Semi-Hydrogenation of Propyne to Propene on CeO2

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Information for Authors

(Revised February, 2015)

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Scope and Editorial Policy

I. General Considerations

ACS Catalysis is an interdisciplinary journal publishing original research on and at the interfaces of heterogeneous catalysis, homogeneous catalysis, and biocatalysis. The journal is devoted to reports of new and original experimental and theoretical research on molecules, macromolecules or materials that are catalytic in nature (exhibiting catalytic turnover), and the catalysts should be characterized to the extent possible by turnover frequencies and fundamental kinetic parameters. Manuscripts that are essentially reporting data or applications of data are, in general, not suitable for publication in *ACS Catalysis*. While papers focusing on catalytic turnover (catalysis) will form the core of the journal, highly impactful papers characterizing catalytic materials or molecules (catalysts) will also be considered. All manuscripts are subject to evaluation by the Editor and/or Associate Editors prior to external peer review, and manuscripts sufficiently lacking in novelty or new insights may be rejected without external peer review. In such instances, these decisions will be made expediently so as to not delay publication elsewhere. Before publication, all manuscripts, including invited contributions, are subject to critical, anonymous peer review. Reviewers are advisory to the Editor. It is understood that the final decision relating to a manuscript's suitability rests solely with the Editor.

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Corresponding authors will receive 50 free electronic reprints via an Electronic Reprint URL. There are no page charges associated with *ACS Catalysis.*

II. Types of Manuscripts

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

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

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

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

D. Reviews are comprehensive, critical examinations of a selected topic, typically over a defined time period. Unsolved problems and emerging areas should be highlighted. A Review should consist of a maximum of 40 pages (approximately 65000 characters) of main text, footnotes, literature citations, tables, and legends. Most Reviews are expected to be substantially shorter in length, but the length will be dictated by the subject matter to some degree. Authors may be invited by the Editor to submit Reviews. Unsolicited Reviews will be considered, as well; however, authors interested in submitting a Review are strongly encouraged to contact the Editor prior to manuscript preparation and submission to seek conditional approval of the proposed review topic. One-page proposals should be sent to the Editor-in-Chief, Christopher Jones (EIC@catalysis.acs.org) for consideration.

E. Viewpoints appear mostly as a result of an invitation from the Editor and will be so designated. Viewpoints may be general commentaries and tutorials of immediate interest to the broad readership. These articles normally will be in highly active research areas, and they are not intended to be reviews of the literature. The author will be asked to provide a clear, concise, and critical status report of the field as an introduction, and the author's own insights or contributions to the field should constitute the main body of the article. Viewpoints will typically range from 3 to 6 journal pages in length. Authors in highly active research fields of broad interest in catalysis are encouraged to propose Viewpoints.

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

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

Additions and Corrections should be submitted by the corresponding author if errors of consequence are detected in the published paper. An addition or correction may be submitted via the ACS Paragon Plus Environment (select "Additions and Corrections" as the manuscript type). All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections may not be submitted by anyone other than the corresponding author of the paper requiring correction. The corresponding author should obtain approval from all coauthors prior to submitting an addition or correction. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work.

III. Functions of Reviewers

The Editor requests the scientific advice of reviewers who are active in the area of research and development covered by the manuscript. The reviewers act only in an advisory capacity, and the final decision concerning a manuscript is the responsibility of the Editor. The reviewers are asked to comment not only on the scientific content but also on the manuscript's suitability for *ACS Catalysis.* With respect to Letters, the reviewers are asked to comment specifically on the urgency of publication. **Authors must suggest, when submitting a manuscript, names and e-mail addresses of at least four scientists who could give a competent and objective evaluation of the work.** All reviews are anonymous, and the reviewing process is most effective if reviewers do not reveal their identities to the authors. An exception arises in connection with a manuscript submitted for publication in the form of a comment on the work of another author. Under such circumstances, the first author will, in general, be allowed to review the communication and to write a rebuttal. The rebuttal and the original communication may be published together in the same issue of the journal.

IV. Revised Manuscripts

A manuscript sent back to an author for revision should be returned to the Editor as soon as possible. The revision deadlines for Articles, Perspectives, Reviews, and Viewpoints are as follows:

- Minor revisions: 21 days
- Major revisions: 45 days
- Reject and resubmit: 90 days

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- Minor revisions: 14 days
- Major revisions: 21 days
- Reject and resubmit: 60 days

If a revision is not received by the given deadline, the manuscript will be considered withdrawn unless an agreement has been reached with the Editor for an extension of the deadline. Revised manuscripts are sometimes sent back to the original reviewers, who are asked to comment on the revisions. If only minor revisions are involved, in most cases, the Editor will examine the revised manuscript in light of the recommendations of the reviewers without seeking further opinions. A letter from the author must accompany the revised manuscript and provide a detailed account of how the author has responded to the reviewer's comments. This letter should include the reviewers' comments and a "point-by-point" response to each, including any changes made, from the authors. The dates of receipt of both the original and revised manuscripts will appear in publication.

Preparation of Manuscripts

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Text

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Schemes. Sequences of reactions are called schemes and should be numbered consecutively with Arabic numerals. Schemes may have brief titles describing their contents and footnotes, if needed, for further detail.

Charts. Groups of structures that do not show reactions are called charts and should be numbered consecutively with Arabic numerals. Charts may have brief titles describing their contents and footnotes, if needed, for further detail.

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

Tables should be numbered consecutively with Arabic numerals and placed in the text near the point of first mention. Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly as narrative, when many numbers must be presented, or when more meaningful interrelationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

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

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

Compound Characterization, Experimental and Computational Data

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

Guidelines for Characterization of Organometallic and Inorganic Compounds.

(a) Routine Compounds

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

(b) Novel or Unexpected Compounds

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

proof of elemental composition, it is acceptable evidence for composition, providing that the results of other physical methods concerning the characterization are conclusive.

(c) Solid State Materials

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

(d) Compounds That Have Not Been Isolated

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

(e) Purity and Yield

The yield and purity of all molecular species must be reported, including the methods used to determine them. The yield of a compound obtained in an NMR tube reaction should be determined using an internal standard.

Guidelines for Characterization of Organic Compounds

(a) Sample Quality

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

(b) Molecular Weight

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

(c) Miscellaneous

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

(d) Intermediates on Solid Phase; Combinatorial Chemistry

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

Kinetic and Equilibrium Data

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

Structural Data for Proteins and Nucleic Acids

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

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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.

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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

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