May

2022

ORGANIC REACTIONS

Editorial Board

Manuscript Guide

ORGANIC REACTIONS MANUSCRIPT GUIDE

Overview

This document provides guidelines for the preparation, submission, and publication of a chapter for Organic Reactions. Supplementary electronic files including Microsoft® Word templates for the outline and rubric, text, and abstract; ChemDraw® stationery files containing the default settings for tables, charts, and text graphics; and an EndNote™ template are also provided via e-mail. All of these documents are available online at the "Author Center" link of the *Organic Reactions Wiki Home Page*: http://organicreactions.org/index.php/Author_Center.

Because Organic Reactions is an ongoing series, style guidelines are less flexible than those for most journals. For the chapter text, we rely primarily on the guidelines provided in The ACS Style Guide,† with some exceptions as noted. However, our graphics styles are very precise and authors must apply the styles described herein to all structures, schemes, and figures.

One of the most valuable features of Organic Reactions is the **Tabular Survey**, which is comprised of examples selected by the author(s) to show the breadth and scope of the chapter's subject reaction. Because of the complexity of the Tabular Survey and the production requirements of our publisher, authors are *required* to prepare table entries using ChemDraw software following carefully established guidelines. The typesetter engaged by our publisher, John Wiley & Sons, will compile these entries into the Tabular Survey once the chapter draft has been approved.

Responsible Editors, who are members of our Editorial Board, are assigned to authors at chapter initiation, and are the authors' principal contacts during the chapter preparation process. Authors should keep their Editors apprised of their progress, as well as of any problems that arise, on a *quarterly* basis. Authors should also become familiar with the sequence of chapter preparation and review as described beginning on page 4.

The end result of the painstaking preparation of such manuscripts is a publication of consistently high quality that continues to serve as a principal reference series. We are grateful to participating authors who help to maintain the high caliber of Organic Reactions.

The Editorial Board of Organic Reactions

---

†Coghill, A. M.; Garson, L. R. *The ACS Style Guide, A Manual for Authors and Editors*, 3rd ed., American Chemical Society: Washington, DC, 2006.

CONTENTS

QUICK START: CHAPTER PREPARATION IN A NUTSHELL **1**
Final Submission Components **1**
Tools Provided (by email and at http://organicreactions.org/index.php/Author_Center) **1**
General Description of Steps **1**
REQUIREMENTS FOR FINAL MANUSCRIPT SUBMISSION **2**
THE CHAPTER PREPARATION PROCESS **4**
THE MANUSCRIPT **6**
Document Settings **6**
Text Sections **6**
Title Page 6
Order and Description of Sections 6
General Format and Style of the Manuscript Text **11**
Specific Conventions for Experimental Procedures **13**
Forms for Data Elements 14
Identifying Text Graphics **15**
Numbering Structures **16**
CITATIONS AND REFERENCES **17**
Reference Management **17**
EndNote **17**
Bibliography Content **17**
GRAPHICS **18**
Style and Format **18**
Stereochemical Depiction **21**
Reporting Regioisomeric and Stereochemical Ratios **23**
Specific Conventions for Text Graphics **24**
Specific Conventions for Table Graphics **24**
THE TABULAR SURVEY **25**
Content **25**
Format **26**
Table Columns 27
Sub-Tables 28
References 28
Footnotes 29

Example Table File with Footnotes 30

APPENDIX I: Checklist for *Organic Reactions* Chapter Authors and Responsible Editors 31

APPENDIX II: Placement and Identification of Text Graphics 34

ChemDraw Files with Insertion Numbers and Titles 34

Sample Text with Insertion Numbers and Embedded Graphics 35

APPENDIX III: Guidelines for Computer-Drawn Text Graphics 36

Annotated Example of a Text Graphic 37

APPENDIX IV: Guidelines for Computer-Drawn Tables and Sub-Tables 38

Sample Table Files 38

How to Prepare the ChemDraw Table Files 41

Construction of Sub-Tables 42

Example 1: Table Entry Sub-Table of Different Conditions 44

Example 2: Table Entry Wherein Substrates/Products Are Simple Analogs and Conditions Differ 45

APPENDIX V: Ligand/Catalyst Numbering 46

APPENDIX VI: Guidelines for Stereochemical Depictions 47

APPENDIX VII: Styles for Selected Abbreviations and Symbols 50

APPENDIX VIII: *The Journal of Organic Chemistry* Standard Abbreviations and Acronyms 51

APPENDIX IX: Chart for Converting % ee into er 54

APPENDIX X: Copy Editing and Proofreading Symbols 55

QUICK START: CHAPTER PREPARATION IN A NUTSHELL

Final Submission Components

1. Abstract, Key Words, Running Header (MS Word document)
2. Manuscript (MS Word document and PDF documents)
3. Text Graphics (ChemDraw files)
4. Tabular Survey (ChemDraw files)
5. References (EndNote library)

Tools Provided *(by email and at http://organicreactions.org/index.php/Author_Center)*

- *Organic Reactions Manuscript Guide* (illustrates all the necessary style and formatting details)
- *Templates:* Outline and Table Organization Rubric / Manuscript Template.dotx / TxGr Stationery.cds (for in-text Schemes and Figures) / Chart Stationery.cdx / Table Stationery.cds / Abstract Template.dotx / Organic Reactions EndNote bibliography template (add this file to the EndNote Styles folder to have the correct format in the bibliography.)
- *Samples:* outline, table organization rubric, text, text graphics, tables and charts, abstract
- *Videos on table file preparation (organicreactions.org)*

General Description of Steps

Working closely with your Responsible Editor (communicate at least every 3 months):

1. Collect references into EndNote.

2. Prepare and submit for approval an Outline of the proposed chapter, the Table Organization Rubric, and sample pages with references, using the templates provided:

- Outline of entire chapter, with complete listing of Tables.
  [This resembles the Table of Contents, but with additional explanation where needed.]
- Table Organization Rubric; also include 1) the planned criteria to select/omit examples and 2) whether the examples in the Schemes will be repeated in the Tables.
  [This will become the Tabular Survey Introduction in the chapter.]
- text sample: 10 pages from Introduction + 10 pages from Mechanism & Stereochemistry
- text graphics sample: 10 inserts from Mechanism & Stereochemistry + 10 inserts from Scope & Limitations
- table samples: 1) 5 filled ChemDraw files from each of two different tables ("TS-I"); then 2) 2 completed tables ("TS-II", incorporating changes from TS-I)

Do not proceed with chapter preparation until samples have been reviewed!

3. Consult the checklist in Appendix I to better understand the requirements for the final product.

4. Write the text and draw the text graphics, choosing reaction examples with complete reaction conditions.

5. Choose examples for the Tabular Survey that best illustrate the scope of the reaction. Order the entries as defined in the approved rubric. Follow the instructional videos (organicreactions.org) and consult the MS Guide to properly construct Table entries and sub-tables.

6. Re-consult the checklist, assemble all the chapter components, and submit the draft for review.

REQUIREMENTS FOR FINAL MANUSCRIPT SUBMISSION

These are the necessary components of a final chapter submission. The checklist in Appendix I has full details and should be consulted during writing.

This section summarizes what the *final submission* package for an *Organic Reactions* chapter must include. The *Organic Reactions Manuscript Guide* is an essential resource that explains how to get to this submission stage. *Please read it carefully* and direct any questions to your Responsible Editor or the Editorial Coordinator.

Use the checklist provided in Appendix I to ensure that the chapter is ready for submission, and include the following components:

1. **Abstract.** The online version of an *Organic Reactions* chapter includes an abstract. The author should submit 10 key words and a 250-word abstract as a Microsoft (MS) Word file to the Responsible Editor with the final copy of the chapter. A shortened title to be used as running header should be submitted by the author if the chapter title exceeds 60 characters, including spaces.

The abstract should be a concise description of the materials in the article and its implications, and should include all key words. Do not include references to other articles, or URLs.

2. **A Single MS Word File of the Manuscript.** The "manuscript" is the chapter text with embedded graphics, and includes the following sections unless the Editor-in-Chief has agreed upon their exclusion.

Title Page (title of chapter, authors' names, affiliations, and addresses, and corresponding author's email address)
Contents (without page numbers; headings should match those in the text and Tables)
Acknowledgments (optional)
Introduction
Mechanism and Stereochemistry
Scope and Limitations
Applications to Synthesis
Comparison with Other Methods
Experimental Conditions (general overview and hazard cautions)
Experimental Procedures
List of Abbreviations
Tabular Survey Introduction

The manuscript sent to the Responsible Editor for review should have insertion numbers *and* embedded text graphics (see Appendix II).

3. **Text Graphics.** These are the ChemDraw files containing all schemes and figures that are in the body of the text. Multiple graphics (interspersed schemes and figures) should be included on a single file page (but do not use multi-page ChemDraw files). Graphics should be numbered sequentially according to their order of appearance in the text, and insertion numbers clearly marked in the upper left corner (see Appendix II). ChemDraw files should be named based on the first insertion number appearing on that file (e.g., TxGr 001-, TxGr 005-, etc.).

4. **References.** The EndNote library must be submitted (.enl and Data folder). The ChemDraw files will contain "unformatted citations" [e.g., {Curti, 2008 #20}], which the *Organic Reactions* Processing Editors will format after typesetting. To ensure that the record numbers (the number after # in the temporary citation) match those in the unformatted citations in the table entries, a single EndNote library should be used for the entire chapter.

5. **Table Entries.** The table entries (ChemDraw files) may be submitted in advance, or together with the manuscript. Authors will receive table galleys to review and revise before receiving page proofs of the entire chapter.

COMMON ERRORS ALERT

Attention authors!

In the remainder of this Guide, *this warning symbol is used to identify the common errors or problems that should be avoided in the preparation of a chapter.*

THE CHAPTER PREPARATION PROCESS

Chapter preparation is a structured process involving the mutual collaboration, coordination, and cooperation of authors and Organic Reactions editors.

Several members of the *Organic Reactions* Editorial Board assist authors with chapter preparation and production. Each chapter is assigned to a Responsible Editor, who serves as liaison with the author. Together with the author, the Responsible Editor ensures that the chemistry is presented accurately with beneficial critical commentary, and in accordance with *Organic Reactions* style. In addition, the Editorial Coordinator checks that the manuscript, text graphics, and tables are in accordance with *Organic Reactions* style, format, and production requirements. Lastly, a secretary to the Editorial Board works with our publisher, John Wiley & Sons, to manage and coordinate chapter submission, page proofs, and publication.

Initially, the Responsible Editor provides the author with samples of an acceptable chapter Outline and Table Organization Rubric, and sample pages for each of the sections (Text, Text Graphics, and Tables). Based on these samples, authors must submit to the Responsible Editor a detailed outline of the material they propose to cover, divided by chapter sections, and including a complete list of proposed Tables. The Table Organization Rubric must also be submitted for approval. The rubric should explain how the examples are divided between Tables and how they are ordered within each Table. *Table entries should be ordered to allow proximity based on similarities in starting material or product structures. Do* ***NOT*** *order by reference or by catalyst.*

Once the chapter Outline and Table Organization Rubric are approved, Text samples, Text Graphics samples, and Table samples must be submitted for review. Table samples must be representative of the content of the Tabular Survey, and the author should not have progressed so far that recommended changes would be oppressive. An author can and should request the review of additional samples if proper formatting is a question at any stage of table construction. Our experience shows that correcting departures from *Organic Reactions* style and format at an early stage can save much time and effort.

Once the proposed Outline, Table Organization Rubric, and all sample pages have been reviewed and approved, the author may proceed to writing the manuscript and assembling the Tables. The author may prepare the manuscript draft either before or after compiling the Tables. This draft, along with the Tabular Survey (created according to the directions provided later in this *Guide*), is submitted to the Responsible Editor who determines if these documents are ready for further review. If so, the Responsible Editor distributes copies of the

text to other editors (and occasionally to outside experts) for review, and then compiles and relays their comments back to the author. The Editorial Coordinator reviews the Tabular Survey for adherence to guidelines and accuracy of organization before arranging for vetting, as noted below. (The Tabular Survey may be submitted in advance of the manuscript draft if prepared as the first step.)

Note that there may be several rounds of reviews involving multiple members of the Editorial Board. *Organic Reactions* seeks to maintain high standards and thus also conducts accuracy checks on the transcription of reactions, both in the Tabular Survey and in the graphics accompanying the text. Chapters with error rates higher than 10% are returned to the author(s) for more thorough reviews and corrections.

Ultimately, an electronic copy of the final, corrected chapter, together with the completed checklist (Appendix I), is submitted to the Responsible Editor, who confirms that all requested revisions have been made, and that the checklist is complete. The Responsible Editor then sends the chapter to the Editorial Coordinator for final processing. The author and editors will have an opportunity to review the processed chapter prior to submission to Wiley for page proofs. Any desired content changes must be made at this stage. Subsequent final review of the page proofs by the author and editors should be limited to the correction of compositing errors.

THE MANUSCRIPT

Document Settings

Use the MS Word template!

An MS Word template with the proper settings is provided by e-mail and is also available online at http://organicreactions.org/index.php/Author_Center.

- ✓ Paper Size: US Letter
- ✓ Font: 12-pt Times New Roman
- ✓ Line-spacing: double
- ✓ Margins: 1 inch top and bottom; 0.75 inch sides
- ✓ Text Alignment: left
- ✓ Use "first line indent"—not tabs—to indent paragraphs.

COMMON ERRORS

The Word template is not used.
Text is justified rather than left-aligned.
Tabs are used to indent paragraphs.

Text Sections

Title Page

Include:

- ✓ Chapter Title
- ✓ Authors' full names, starting with the corresponding author
- ✓ Authors' affiliation, department, university or company, city, state, and country (in English)
- ✓ Dedication (only allowed in memoriam; contact the Editorial Coordinator for format)
- ✓ Corresponding author's e-mail address in the first page footer

Order and Description of Sections

Contents should match the actual text headings and subheadings.

CONTENTS

List:

- ✓ Headings and subheadings used in the text
- ✓ Experimental Procedures, including product name and generalized description
- ✓ Numbers and titles of all Charts and Tables in the Tabular Survey
- ✓ Do not include page numbers

ACKNOWLEDGMENTS

(*Optional*)

INTRODUCTION

Be concise!

- ✓ Define and illustrate the reaction.
- ✓ Define the scope, and indicate limitations to the coverage.
- ✓ Limit the citation of chemists' names and historical background. *Do not* include a chronological development or early history of the reaction.
- ✓ Provide references to any previous reviews of the reaction.

COMMON ERRORS

Too much historical background is provided.

Mechanistic discussions and implications are included here rather than in the next section.

MECHANISM AND STEREOCHEMISTRY

(*May be separated into two sections*.)

- ✓ Briefly and critically discuss *current* mechanistic models, avoiding historical development. Discuss mechanistic issues that have not been fully addressed.
- ✓ Discuss factors affecting the stereochemical course of the reaction, including shortcomings in selectivity.
- ✓ Use carefully selected graphic illustrations to illustrate the origin of selectivity.

SCOPE AND LIMITATIONS

(*This section is the backbone of the text discussion, and must not only be accurate in content, but also scholarly in presentation.*)

Emphasize content and double-check for scientific accuracy and faithful transcription of information.

- ✓ Provide a *critical analysis* of the current status of the reaction.
- ✓ Limit citation of chemists' names to those who discovered the reaction or an important modification of it. Exclude dates.
- ✓ Provide information that will help a chemist select conditions for using the reaction effectively.
- ✓ Provide incisive commentary explaining the rationale for selection of certain reaction protocols amidst a variety of options.
- ✓ Use an adequate number of examples on which to base a premise, BUT *do not* present a running catalog of literature reports.

- ✓ Illustrate all phases of the reaction with graphics.
- ✓ Select text graphics judiciously, using reactions for which complete experimental details have been provided, including an isolated yield. *In addition to substrate and product structures, the depicted reactions must include all reagents and their stoichiometric amounts, solvents, temperature, time, isolated yield, and regioisomeric and stereochemical ratios*.
- ✓ Any reaction illustrated in a text graphic or table entry that potentially creates isomers should specify an appropriate selectivity metric (dr, er, (*E*)/(*Z*), site selectivity, etc.) and use the appropriate single/wavy/wedge/hash bond, as described in Appendix VI.
- ✓ Provide a citation for *every* graphic.
- ✓ Include *current* limitations on the scope of the reaction.
- ✓ Suggest new applications or extensions of the reaction.

COMMON ERRORS

Discussion lacks critical commentary.
Reaction examples are excessive.
Reaction graphic conditions are incomplete.
Reaction graphics do not illustrate associated text.
Reaction graphics are inaccurate.
The text does not provide a citation for the reaction graphic.

APPLICATIONS TO SYNTHESIS

- ✓ Include a few examples of important syntheses in which the reaction has been used to prepare natural products and other compounds of value such as pharmaceutical or agricultural products.
- ✓ Choose examples that showcase different aspects of the reaction rather than providing an exhaustive review.

COMPARISON WITH OTHER METHODS

- ✓ Describe other synthetic approaches to the same products.
- ✓ Compare other approaches (advantages and disadvantages) to preparing the functional-group transformation outlined in the subject reaction.
- ✓ In addition to substrate and product structures, the depicted reactions must include all reagents and their stoichiometric amounts, solvents, temperature, time, isolated yield, and regioisomeric and stereochemical ratios.

- ✓ Cross-reference with specific examples in Scope and Limitations for comparison.

EXPERIMENTAL CONDITIONS

- ✓ Identify significant hazards and safety precautions. Set warnings in italics, preceded with "CAUTION:".
- ✓ Provide a laboratory procedure for handling and destroying particularly hazardous reagents, starting materials, or products. Include relevant MSDS or other references.
- ✓ Comment on preferred catalysts, solvents, and other conditions.
- ✓ Describe any unusual techniques for handling reagents or isolating products.

EXPERIMENTAL PROCEDURES

- ✓ Include enough procedures to illustrate *significant* applications and variations of the reaction, being selective so as to minimize redundancy.
- ✓ Select examples that provide the most detailed description of the experiment for that example, including stoichiometry of all reactants and reagents, isolated yields, and thorough characterization of the products.
- ✓ Include a large-scale preparation if available in the literature.
- ✓ Each procedure title should include the product name, and in square brackets a description of the reaction sub-type.

COMMON ERRORS

Text description does not match information shown in the associated graphic reaction.
Analytical data are incomplete and/or do not adhere to OR style.
Data are presented out-of-order (see page 13).
Data presentation is inconsistent within the section.
Examples do not illustrate the breadth of possible reagents and procedures.

LIST OF ABBREVIATIONS

- ✓ Provide a list of abbreviations used in the Tables, Text, and Text Graphics if they are not included in "*The Journal of Organic Chemistry* Standard Abbreviations and Acronyms" (Appendix VIII). The Responsible Editor should approve uncommon abbreviations in advance.

TABULAR SURVEY

(The following points refer to the introduction that must precede the Tabular Survey. Guidelines for the Tabular Survey itself appear later in this document.)

- ✓ Provide the cutoff date for the literature survey.
- ✓ State whether or not the Tables include all the examples in the literature, or are selective examples.
- ✓ State whether or not the reactions in the text graphics (Schemes) are repeated in the Tables. *Note that <u>either all or none</u> of the in-text reactions (except those in the Comparison with Other Methods section) should be repeated in the Tables.*

- ✓ Describe the organization of the Tabular Survey: Table divisions should be based on substrate (or product) structures, *NOT* on catalyst/ligand used.
  - ➢ 1. How the substrates are divided between the Tables
  - ➢ 2. How the substrates are ordered within each carbon count
  - ➢ 3. How multiple entries for a particular substrate are ordered

- ✓ Identify structural elements that are not included in the carbon count of the substrate.
- ✓ Explain the use of charts, if any.
- ✓ Explain any unusual conventions used in the Tabular Survey.

This introduction to the Tabular Survey ends the text portion of the manuscript. The Tabular Survey itself consists of ChemDraw files comprised of all examples necessary to show the breadth and scope of the title reaction. See page 25 and Appendix IV for a detailed description.

General Format and Style of the Manuscript Text

Consult the ACS Style Guide *in addition to the* Organic Reactions Manuscript Guide*!*

For grammatical style and formatting of the chapter text, *Organic Reactions* defers to the *ACS Style Guide*, *3rd edition*. Exceptions or emphases are noted below. Authors should consult the *ACS Style Guide,* especially with reference to verb tense, punctuation, use of en- and em-dashes, hyphenation, and italicization.

✓ Arrange the chapter headings as illustrated.

The following examples show the arrangement and format for (1) a heading with three subheadings, and (2) a heading with four subheadings. Should more than four subheadings be required, please contact the Editorial Coordinator.

Check that headings and sub-headings in the text agree with those listed in the "Contents".

(3 subheadings)

SCOPE AND LIMITATIONS
Reductive Desulfonylation

Reductive Desulfonylations by Active Metals and Salts. (Text follows on same line.) A major disadvantage of the use of metals and their salts, particularly on a large scale…

Use of Alkali Metals in Ammonia. (Text follows on same line.) The reductive desulfonylation process with…

(4 subheadings)

SCOPE AND LIMITATIONS
Grignard-Derived Organocopper Reagents

Copper-Catalyzed Reactions of RMgX [Do not use unless you need four or more levels of subheadings.]
(Begin text, if any, on new line.)

Substitution Reactions. (Text follows on same line.) The pros and cons of using Grignard…

Epoxides. (Text follows on same line.) Ring opening of epoxides can be achieved…

✓ ***NOTE WELL!*** *Use the passive voice in present or past tense throughout the text, but use the past tense for the Experimental Procedures.*

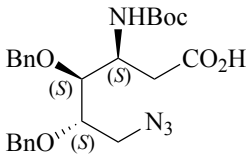
Exception to ACS Style Guide!

- ✓ Unlike the convention given in *The ACS Style Guide*, *always* use italic type for positional, stereochemical, configurational, and descriptive structural prefixes *whether or not* they appear with the chemical name or formula. A hyphen must be used after the prefix in complete chemical names. The use of a hyphen after all such prefixes not associated with full chemical names is at the author's discretion, but usage must be consistent throughout the chapter.

  trans isomer, *cis*-propenylcyclohexane
  "…the hydrogens at the ring fusion have a *cis* relationship."

  (*R*), (*S*), (*Z*), and (*E*) are *always italicized and in parentheses*. The parentheses themselves, however, are not italicized.

  (*R*) and (*S*) isomers, (*Z*) alkenes
  (4*R*)-3,4-dimethyl-4-phenylhexan-2-one
  (*R*)-**21**, where the bold number represents a specific compound
  (*E*,*E*)/(*E*,*Z*)/(*Z*,*Z*) = 45:43:12



R	Yield (%)	(*E*)/(*Z*)
Me	13	2:1
i-Pr	49	4:1
Ph	41	1:2

Catalyst	Yield (%)	er
(*R*,*S*)-**C3**	76	95.0:5.0
(*S*,*S*)-**C14**	55	99.5:0.5

- ✓ Unlike the convention given in *The ACS Style Guide*, *always* use italic type for element symbols denoting attachment to an atom or site of ligation, *and* when used as an adjective or noun denoting a type of reaction.

  N-acetyl, *N*-acetylation

- ✓ In general, use names, not formulas, for common chemicals in the text. However, if a common chemical with a long name is mentioned frequently, a trivial name or acronym can be used; it should be defined at the first use, for example:

  diglyme (diethylene glycol dimethyl ether)
  TBDPS (*tert*-butyldiphenylsilyl)

- ✓ Formulas of complex chemicals can be used instead of their names: $LiAlH(O\textit{t}\text{-}Bu)_3$ rather than lithium tri(*tert*-butyloxy)aluminum hydride.

- ✓ Use a serial comma before "and" or "or" in a list of 3 or more items. For example, "The reaction occurs with aldehydes, ketones, and carboxylic acids."

Specific Conventions for Experimental Procedures

- ✓ Illustrate the procedure with a reaction graphic that precedes it.
- ✓ Follow the name of the product with a short phrase identifying the reaction type:

  Methyl 3-Amino-2-thioformylcrotonate [Thioformylation of an Enamine].[30] A solution of $POCl_3$ (0.5 mL, 5.5 mmol, 1.1 eq) in DMF (1.5 mL) was added…
- ✓ Use past tense for the Experimental Procedures section.
- ✓ Use consistent language and format for all the experimental procedures so that the section is cohesive.
- ✓ Use formulas/abbreviations for common solvents such as Et_2O, EtOAc, THF, DMF, DMSO, CH_2Cl_2, $CHCl_3$, etc., rather than full chemical names.
- ✓ Abbreviate units of time (s, min, h, d), "room temperature" (rt), and equivalents (eq).
- ✓ Give actual and percent yields and important physical constants of the product.
- ✓ Use this order for analytical data: bp or mp; t_R or R_f data (HPLC, TLC, GC); specific rotation; UV; IR; ^{1}H NMR; ^{13}C NMR; mass spectra; HRMS. Elemental analysis.
- ✓ Separate data sets using a semicolon. Use a period after the data preceding combustion analysis.
- ✓ Chemical shift data should follow the same order, either ascending or descending, from one procedure to the next.
- ✓ Include *Organic Syntheses* procedures as a reference to the primary source, without detailing the procedure, except to state the scale and yield. Prepare a graphic that includes reaction conditions.

  8-[2-(Triethoxysilyl)ethyl]-1-tetralone [Ketone-Directed C–H Alkylation]. This procedure was published in *Organic Syntheses*.{Kakiuchi, 2003 #373} The reaction was performed on 500 g scale, and provided the title product in 92% yield.

Forms for Data Elements

- ✓ mp 82 °C
- ✓ HPLC t_R (*R*) 7.7 min (68%), t_R (*S*) 8.9 min (32%) (Chiralpak OJ, 1% *i*-PrOH/hexanes, 2.0 mL/min, 220 nm, 40 °C)
- ✓ TLC R_f 0.24 (EtOAc/hexanes, 2:1)
- ✓ GC t_R (major) 63.14 min, t_R (minor) 64.28 min (Chirasil-dex; 80 to 100 ºC, 5 ºC/min, then 100 to 180 ºC, 0.5 ºC/min, 15 psi)
- ✓ $[\alpha]_D^{25}$ + 85.0 (*c* 0.02, MeOH)
- ✓ UV (hexanes) λ_{max} (ε): 250 (1070)
- ✓ FTIR (NaCl) 1824, 1454, 1248, 1102, 942 cm^{-1}
- ✓ ^1H NMR (400 MHz, $CDCl_3$) δ 7.30–7.10 (m, 5H), 5.29 (dd, *J* = 6.4, 8.5 Hz, 1H), 5.13 (d, *J* = 14.9 Hz, 1H)
  - o (shifts to 2 decimal places and coupling constants to 1 decimal place)
- ✓ ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.3, 135.4, 128.7
  - o (shifts to one decimal place)
- ✓ LRMS–CI (NH_3) (*m/z*): $[M + H]^+$ 423, 367, 349
- ✓ HRMS–ESI (*m/z*): $[M + Na]^+$ calcd for $C_{13}H_{16}O_2Na$, 227.1048; found, 227.1046.
  - o (formula should be of the detected compound; e.g., include Na if detected as the Na salt)
- ✓ Anal. Calcd for $C_{18}H_{15}F_3O_2$: C, 67.50; H, 4.72. Found: C, 67.52; H, 4.80.

Identifying Text Graphics

Use insertion numbers AND graphics in the text. See Appendix II.

Appendix II *shows how text graphics files should look, how they are labeled, and how insert numbers are used in the text.*

Appendix III *includes an annotated example of a Scheme. Examine it before starting!*

- ✓ Each text graphic must have a citation of only the reference from which the example is taken. If more references are relevant to the statement, the remaining citations should be placed at the end of the sentence. For example:

  "Stereogenic, quaternary centers can be formed by this method (Scheme 34);[53] the reaction is selective for vinylogous amides with aryl alkynes, and is selective for lactams when alkyl alkynes are used.[53,54]"
- ✓ Add the term "Scheme" or "Figure" below each graphic *in the ChemDraw file*. (Note that *Organic Reactions* no longer uses the term "Equation".)

> *Schemes*: All reactions, including those showing one or more intermediates, and/or reactants or conditions containing variables (Ar, R, X). Schemes do not have legends.
>
> *Figures*: Graphics that usually do not have reaction arrows. Figures must include a legend.

- ✓ Assign an insertion number to each graphic and add it to the ChemDraw file (top left corner of each graphic) and the Word file (under the associated paragraph). Embed the text graphic (schemes and figures) below the typed insertion number in the text file.
- ✓ Assign numbers to schemes and figures in sequence, and use the following formats:

  text: Scheme 1; graphic: **Scheme 1**
  text: Fig. 1 or (Fig. 1), depending on context;
  graphic: **Figure 1.** Legend.
  All figures must have legends written in the ChemDraw file.

- ✓ Use tables (as portrait .cdx files) in the text only if essential and identify them with capital letters (e.g., Table A) to distinguish them from those in the Tabular Survey.

COMMON ERRORS

Insertion numbers are not assigned in the ChemDraw files and/or not included in the text.
"Schemes" are labeled as "Equations".
Figures do not include legends.
Text graphics titles are in the Word file instead of the ChemDraw file.

Numbering Structures

✓ Do not use Roman Numerals in the text graphics.

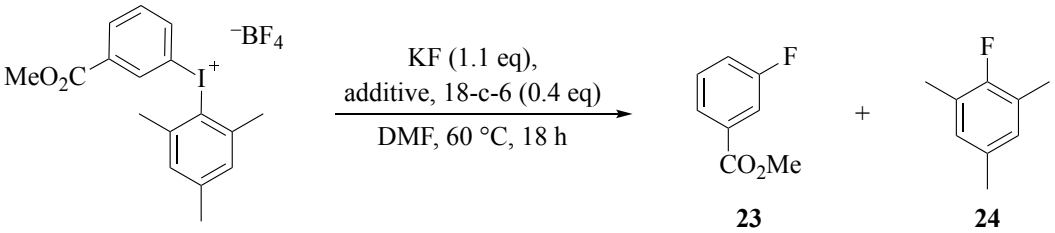
If the discussion requires reference to a structure in a text graphic, identify the structure with a *unique* **boldface** Arabic numeral and use the same boldface numeral in the text. Structure numbers should be assigned in numerical sequence in order of appearance in the text graphics, beginning with the number **1**.

The number should be used with a descriptive noun like 'keto ester **13**' or 'furyl carbinol **15**'. Avoid the use of generalized descriptors like 'compound **13**'. The descriptive noun can be omitted if deemed repetitive in the paragraph. Place the number in parentheses only if the structure is completely named, like '3-methylcyclohexanone (**25**)'.

✓ *DO NOT number every structure.* Number only those that will facilitate the discussion. Likewise, *DO NOT number a structure if that number does not appear in the text.* The only exceptions to this rule are

(1) numbers used to identify repeated ligands/catalysts
[marked as **lig.x**, **cat.x**, etc.]

(2) numbers used to identify products in sub-table ratios and yields.



23 **24**

Additive	Yield (%) **23** + **24**	**23**/**24**	Ref.
—	64	50:50	{Cabrele, 2016 #76}
$Cu(OTf)_2$ (0.2 eq)	73	94:6	{D'Auria, 2000 #17}

✓ See Appendix V for additional important instructions for ligand numbering.

COMMON ERRORS

Compound numbers are assigned to every structure, or are overused.
Tables are used in the text where one or two examples would suffice.

CITATIONS AND REFERENCES

Reference Management

DO NOT use the MS Word footnote/endnote feature for entering references in the manuscript. The resulting field codes cannot be converted to static text, which is a requirement for submission for publication.

Organic Reactions requires authors to use EndNote Desktop software. *Do not use EndNote Online because it cannot create temporary citations for ChemDraw.*

Authors are recommended to enroll in the free 30-day trial period available at endnote.com. Purchase of student copies and upgrades from previous versions are available as less expensive options. Each license may be used on 3 computers by the same person/registered email. *Organic Reactions* can reimburse up to $200 per chapter to offset the purchase of reference management software upon submission of a publishable chapter. The receipt for the purchase of EndNote should be emailed to the *Organic Reactions* Treasurer, Dr. Jeffery Press, jpressorxn@aol.com.

EndNote

- ✓ Database search results can be transferred directly into an EndNote library.
- ✓ Insert citations into the Text with the Cite While You Write function.
- ✓ Put reference citations in the text *after* any punctuation.
- ✓ Insert citations into the Table entries by dragging the reference into the ChemDraw file, or by copy/paste into a text box.
- ✓ Note that *Organic Reactions* has a process for creating the bibliography from the temporary citations in the ChemDraw files. EndNote cannot create a bibliography from .cdx files.
- ✓ A single EN Library must be used for the entire chapter to ensure that Record Numbers (the number after # in the temporary citation) match those in the Library. Therefore, it is highly recommended that a single author be designated as the library manager.

Bibliography Content

- ✓ An Organic Reactions Style template is included in the initial template folder sent by the Editorial Coordinator.
- ✓ *The EndNote Library* must be included *when the chapter is submitted for processing. The Record Numbers must match those in the Table citations.*

GRAPHICS

Style and Format

ChemDraw files must be submitted for both the text graphics and the tables.

Three very important ChemDraw stationery files were provided at chapter initiation. *Use these stationery files as templates for the preparation of text and table graphics.*

USE THESE FILES!

OR TxGr Stationery.cds

OR Chart Stationery.cds

OR Table Stationery.cds

Default document settings can be viewed from the menu: File/Document Settings…

COMMON ERRORS

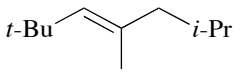
Table pages prepared by multiple coauthors show inconsistent structure representations, expression of conditions, abbreviations, etc.

The following guidelines apply to formulas and structures in both text graphics and tables. When more than one style is acceptable, choose one and use it consistently throughout the chapter. Also see the sections "Specific Conventions for Text Graphics" and "Specific Conventions for Tables".

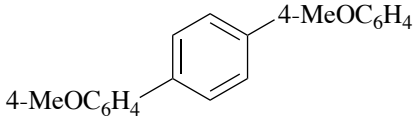
See Appendix VII for preferred abbreviations and keyboard shortcuts for symbols

- ✓ A list of approved abbreviations published by the *Journal of Organic Chemistry* is available at http://pubs.acs.org/userimages/ContentEditor/1218717864819/joceah_abbreviations.pdf and is reproduced in Appendix VIII. Define only those abbreviations that do not appear in the *JOC* list.
- ✓ Use abbreviations or acronyms for long chemical names in conditions.
- ✓ Number sequential steps using 1., 2., etc., not 1), 2), etc.
- ✓ In both the text graphics and the Tabular Survey, *reaction details must include the stoichiometry of the reactants and reagents, solvent, temperature, time, yield, and regioisomeric and stereochemical ratios.*
- ✓ Report catalyst, solvent, conditions (such as pressure or MW), temperature, and time, **in that order**.
- ✓ Abbreviate units of time (s, min, h, d), "room temperature" (rt), and equivalents (eq) in both Text Graphics and Tables.
- ✓ Report stereoselectivities as er and dr (not % ee and % de). The enantiomeric ratio should add up to 100.

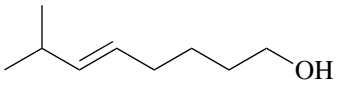
- ✓ Include the er and dr of starting materials and products, when reported in the primary literature.
- ✓ Place yields in parentheses with the % sign; e.g., (92%).
- ✓ Use (0%) for products that are not formed; (—) for no yield reported.
- ✓ Use "heat", not "Δ"; *however*, specify temperature whenever possible.
- ✓ Use the following notation for microwave conditions: MW (300 W), 100 ºC, 10 min
- ✓ Use the following notation for solvent mixtures: $MeCN/CH_2Cl_2$ (3:1)
- ✓ Use an en-dash for minus signs, optical rotation, and number ranges (e.g., temp, time, yields).
- ✓ Do not use charge signs on simple salts.
- ✓ Use charge signs, not circled, on complex salts.
- ✓ Use the ChemDraw radical dot for radicals.
- ✓ Use the 'open bond' to represent methyl attached to carbon.
- ✓ Use "Me" for methyl attached to a heteroatom.
- ✓ Use R^1, R^2, R^3; not R, R^1, R^2 or R_1, R_2, R_3 or R, R', R''
- ✓ Use X only for (pseudo)halogen, HX for (pseudo)halogen acid.
- ✓ Use Y, Z for other generics, such as nucleophiles or leaving groups.
- ✓ Use the numeric (2-, 3-, 4-) rather than the alternative (*o*-, *m*-, *p*-) isomer indicator system.
- ✓ Place isomer indicators before a substituent.



Ar = 2-MeO-4-HOC_6H_3

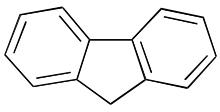


- ✓ Except for captions defining "R–" groups, use line drawings, not linear formulas.

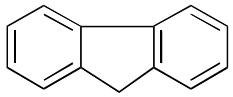


NOT (*E*)-$CH_3CH(CH_3)CH{=}CH(CH_2)_3CH_2OH$

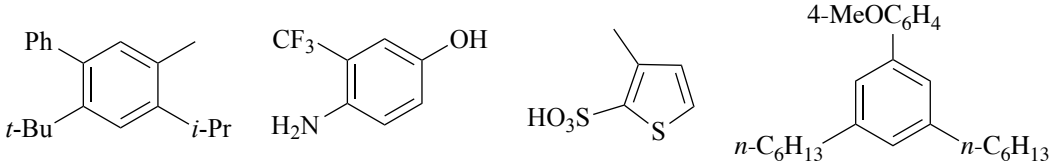
- ✓ Use Kekulé bonds in aromatic rings. The inscribed circle or ellipse should be used only for ions, complexes, and ferrocene-type compounds.
- ✓ Use the regular pentagon, not the "log cabin," for 5-membered rings.



NOT

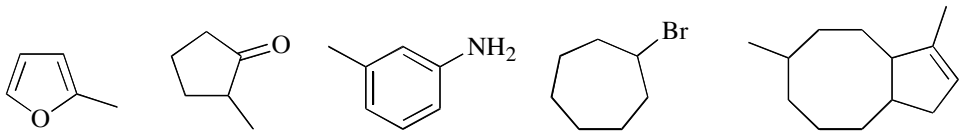


- ✓ Direct bonds to rings toward the center of a regular polygon unless crowding makes this impossible. (Clicking with the ChemDraw bond tool on an atom in a ring will automatically put the new bond in the correct orientation.)
- ✓ If it is necessary to save space or relieve crowding, formula designations for common cyclic and heterocyclic rings can be used.
- ✓ Draw hydrocarbon and halohydrocarbon substituents on the left sides of rings in the direct form. Draw other substituents to show the mode of attachment.



- ✓ In general, set 6-membered and heterocyclic rings on a ring point; set other rings on a base.

Check with the Editorial Coordinator if correct structure orientations are in question.



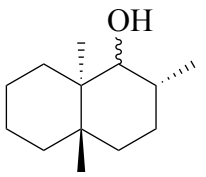
Orientation rules may be modified if the structure is complex, the rings are not involved in the chemical transformation, or orientation is dictated by a consistent representation of a reactant.

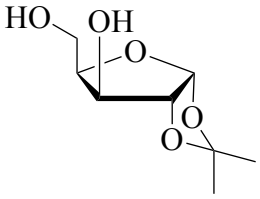
- ✓ Wherever possible, maintain a similar orientation between the structure(s) of the starting material(s) and the structure(s) of the product(s).
- ✓ Scale structures to 85% of the original (but *do not* scale atom labels) if drawn over arrows or shown in conditions, included in sub-tables, or used to define R groups underneath structures.

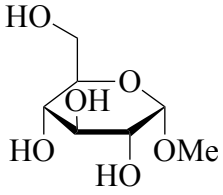
Stereochemical Depiction

- ✓ Denote configurations with the conventions shown in the decalol below. The stereostructure of sugars can be shown as in the following examples.

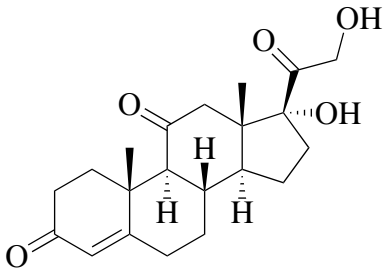
Do not use solid dots or bar lines to denote configuration at ring junctions!

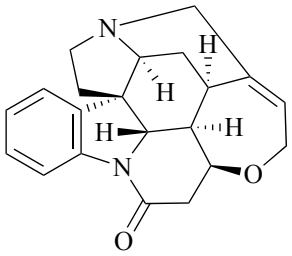






- ✓ Define the configuration of all stereocenters in polycyclic compounds.



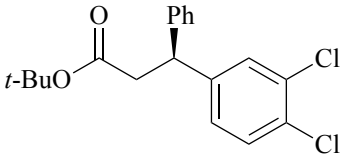


- ✓ See the next pages about the usage of wedged/hashed bonds versus straight bonds versus wavy bonds, and reporting isomer ratios.

Use the bonds as described below, whether or not they match the bond usage in the reference. Authors should determine the appropriate bond to use based on the data provided in the text and Supporting Information of the reference rather than reporting the depiction in the graphic of the reference.

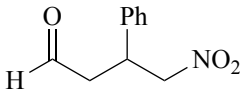
✓ *Organic Reactions* uses the following guidelines to depict isomers.

- Draw the major isomer when the product is a mixture of isomers with specified composition and known configuration. Structures of minor isomers may be included if necessary for clarity.



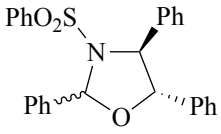
(88%) er = 88.0:12.0

- Use a straight line for the key bond when the product is a single isomer or a mixture of isomers with specified composition, but no configurational assignment. A structure with 1 stereocenter denoting a racemic mixture should use straight-line bonds.



(93%) er = 61.5:38.5

- Use a wavy line for the key bond when the product is a mixture of unknown composition.



(82%)

✓ See Appendix VI for additional examples of stereochemical depictions.

Reporting Regioisomeric and Stereochemical Ratios

Report **all available ratios** for regioisomers, diastereomers, and enantiomers in the text graphics and table entries. The dr/er/(*E*)-(*Z*) ratios for starting materials should also be included if the ratios can be affected by the reaction.

- If a dr is not reported, it is not necessary to add "dr —", unless it's part of a subtable column.

- If the text of a reference states that a "single diastereomer" is obtained:

    - If the dr was determined (check the Experimental section and the Supporting Information), report the dr instead of "single isomer".

    - If the dr was not published, but the reference states that only a "single isomer" was obtained as determined by ^{1}H NMR, report dr ≥ 95:5 instead of "single isomer"; if by HPLC/GC, report dr ≥ 99:1.
        - *Warning*: do not assume these ratios simply based on the fact that spectroscopic characterization is published for the major isomer. The minor isomer may have been separated.

    - If no additional information is available, the term used in the reference (e.g., "single diastereomer") in quotation marks may be used.

- Analogous rules apply to reporting regioisomeric and enantiomeric ratios.

    - It is not necessary to report that a starting material is racemic.

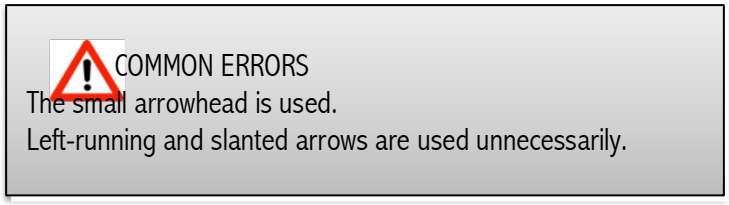
- When applicable, the following statements should be added to the Introduction and Tabular Survey Introduction sections:

    - The term "single isomer" is only used when reported as such in the literature without additional information.

    - Any missing selectivity data reflects their omission in the primary literature.

Specific Conventions for Text Graphics

- ✓ See Appendix II and Appendix III for helpful examples.
- ✓ Although the text graphics should be inserted into the text file, remember that the native .cdx files also have to be submitted.
- ✓ Place non-isolable, reactive intermediates in square brackets.
- ✓ Use the medium-headed arrow, even for cyclic mechanisms.
- ✓ Do not use slanted arrows and minimize the use of left-running arrows. Schemes that illustrate different results from different reagents or conditions should be drawn with orthogonal lines and arrows.
- ✓ Do not capitalize words over or under arrows.
- ✓ Center-align conditions over/under arrows.
  Exception: left-align numbered steps.
- ✓ Do not use Roman numerals; see page 16 for details about numbering.
- ✓ Limited sub-tables may be used to illustrate the scope of a reaction shown in a scheme. Consult Appendix IV for proper sub-table format.



Specific Conventions for Table Graphics

- ✓ Unlike the Text Graphics, the Table .cdx files should never be inserted into a Word file.
- ✓ Capitalize the first word of the "Conditions" (except rt).
- ✓ Report reactant (if not in a separate column), catalyst, solvent, conditions (such as pressure or MW), temperature, and time, in that order.
- ✓ If the conditions require more than one print line, the 2nd and succeeding lines should be indented by 2 spaces. Use a comma at the end of each line.
- ✓ For numbered steps, indent the lines between the numbered steps by 4 spaces.

n-$C_6F_{13}I$ (1.1 eq), Cu (2.3 eq), DMSO, 125–130 °C, 5 h	1. MeI (2.2 eq), TDAE (2.2 eq), DMF, –30 °C, 0.5 h; then rt, o/n 2. HCl or H_2SO_4, H_2O, rt, 5 min

THE TABULAR SURVEY

Content

Obtain approval for table organization from the Responsible Editor. Samples are imperative!

The Tabular Survey should present the breadth and scope of the title reaction. The Tabular Survey is no longer required to be an encyclopedic record of reactions and as such does not need to delineate every single example, but rather provide a survey of what is deemed most useful and significant to the reader. The Author and Responsible Editor will decide on the size, scope, and organization of the Tables required to provide important examples pertinent to the title reaction with ultimate Executive Editor and Editor-in-Chief approval. Although some non-optimal reactions may be included in the Tabular Survey, only the optimal conditions in each study should be reported in general. The survey should be current up to six months before submission. Authors should be prepared to update tables when necessary to make sure that the content is current.

COMMON ERRORS

Table samples are not submitted in accordance with timelines.
Table organization is neither approved nor optimized.
Insufficient information is provided for reaction conditions.
Tables are not vetted for accuracy; reactions are transcribed incorrectly.

- ✓ In both the text graphics and the Tabular Survey, *reaction details must include the stoichiometry of the reactants and reagents, solvent, temperature, time, yield, and isomeric ratios.* (Because these values are not always reported in the primary literature, make a note in the introduction to the Tabular Survey that if the data is not shown in the tables, it was not available from the original publication.)
- ✓ If yields of isolated products are not available from the primary literature, indicate the yield with an em-dash in parentheses: (—). Yields determined using analytical methods, such as GC and NMR, may be reported, but must be labeled as such. For example, (86%) by NMR.
- ✓ Use **charts** at the beginning of the Tabular Survey to depict repeated structures of complex ligands, catalysts, or other reagents. See Appendix V for numbering instructions.
- ✓ Organization of the entries should facilitate logical search and retrieval of reactions by the reader, and allow for reactions resulting in the same or analogous products to appear in proximity, *therefore…*
- ✓ Table organization should be predicated on starting material or product structure, NOT on catalyst or reagent or conditions.

- ✓ Generally, table entries are organized by carbon count of the *substrate*. When such organization of the Tabular Survey is not desirable, the author must have approval from the Responsible Editor and the Editor-in-Chief for an alternative organization.
- ✓ In order to place analogous substrates in proximity, the carbon count should exclude small groups on heteroatoms, protecting groups, and chiral auxiliaries.
- ✓ Substrates are ordered by carbon count (primary ordering), and within each carbon count the substrates should be ordered consistently by other measures (e.g., oxidation state, ring size, etc.) (secondary ordering).
- ✓ Multiple entries for a single substrate should be placed together. If the substrate reacts with a variety of co-reactants, the co-reactants should be ordered consistently (tertiary ordering).
- ✓ *Unless precluded by the secondary/tertiary ordering*, arrange entries of the same substrate by ascending equivalents used of the substrate, starting with the substrate as the limiting reagent (1.0 eq).
- ✓ All examples from optimization studies should **NOT** be included. Instead, choose the best 1–3 conditions to exemplify the point of the study.
- ✓ Discuss all of these issues with the Responsible Editor so that they are aware of any issues that may be flagged during the review process.

Format

Authors are referred to the *Organic Reactions Wiki Home Page* to download a PowerPoint tutorial or view YouTube videos on table and sub-table preparation: http://organicreactions.org/index.php/Author_Center.

- ✓ Carefully read the tutorial and faithfully follow the instructions. The contents of the tutorial are reproduced in Appendix IV for easy reference.
- ✓ *DO NOT use the multi-page feature ("poster") in ChemDraw.* Each page of table entries must be a *separate* ChemDraw file. *A 2-row page may only be used for a sub-table in the Tabular Survey that is larger than 1 page.*
- ✓ *DO NOT attempt to duplicate the printed page of a final OR volume.* Wiley's compositor will apply the necessary formatting.

Table Columns

Carbon Count

- ✓ Show the carbon count for every entry. See the section beginning on page 41 in Appendix IV for suggested exclusions from the count.

Substrate/Starting Material

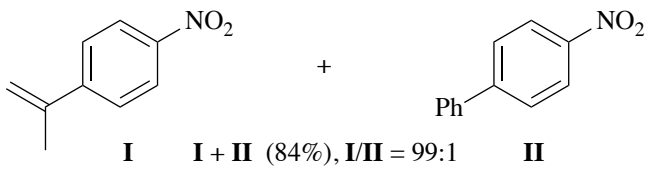
- ✓ Repeat the structure for the starting material in every entry.
- ✓ Orient structures of starting materials and products similarly.

Conditions

- ✓ Repeat the conditions for each entry.
- ✓ Use an em-dash in the column if conditions are not reported.
- ✓ Report catalyst, solvent, conditions (such as pressure or MW), temperature, and time, in that order.

Product(s) and Yield(s)

- ✓ Orient structures of starting materials and products similarly.
- ✓ If there is not adequate space within a column for multiple products, use 2nd, 3rd, etc. lines, indenting a few spaces from the initial product(s).
- ✓ Use a plus sign between multiple products.
- ✓ If there is more than one large product, draw partial structures using a bracket, { or }, to indicate the missing portion.
- ✓ Write yields in parentheses, e.g., (80%), and enter them following each product. Do not enter yields in a separate vertical column unless they are part of a sub-table within an entry. Use the notation "(—)" for unreported yields and use (0%) if the product was not observed. Yield columns in sub-tables have the heading "Yield (%)", and thus the values are written without parentheses.
- ✓ Do not set ratios of products and isomers in parentheses.
- ✓ Use “er” instead of “% ee”, and specify absolute configuration. See Appendix IX for a conversion chart.
- ✓ Use Roman numerals to show combined yield and product ratios for two or more products. Do not continue the Roman numeric sequence beyond one set of entries: restart with **I** for each entry. The plus sign and slash are set in plain, not boldface, type.



I **I** + **II** (84%), **I**/**II** = 99:1 **II**

Important Note on the Use of Sub-Tables

Because the content of *Organic Reactions* is ultimately entered into an online structure-searchable database, the use of sub-tables in individual table entries should be limited to those examples where the substrates and/or products are simple analogs, or where the substrate and product(s) remain the same and conditions differ only slightly (e.g., same reagents, but different catalysts, times, or temperatures). The use of sub-tables is recommended for analysis of the effects of simple structural changes or alteration of conditions on the outcome of a reaction, if arrangement by carbon count separates the related entries.

Sub-Tables

Complete instructions for constructing sub-tables are in Appendix IV.

See Appendix IV for Tabular Survey sub-table examples.

- ✓ Sub-table entries should be ordered by the same logic as used for ordering of the table entries, except in the text graphics where the entries may be better organized based on the discussion.
- ✓ In both the Tabular Survey and text graphics, if a sub-table contains entries from multiple references, add a reference column to the sub-table.
- ✓ Draw substituents with attachment points on the right except for hydrocarbon substituents (and CX_3, X = halogen), which are drawn in direct form. (See page 43 for proper orientation of some common groups.)
- ✓ Use an en-dash after potentially ambiguous R groups such as cyano and isocyano (NC–, CN–).

References

- ✓ Use EndNote citations for table entries, as described earlier in the section beginning on page 17.
- ✓ Each entry must have a reference. If there is more than one reference for an entry, the first reference should be the one on which the entry is based, regardless of numerical order.
- ✓ When a sub-table is constructed from the same reference, use the reference number once, and align it with the structures. If different references contribute to the sub-table, show each reference in the reference column in line with the corresponding sub-table entry.

Footnotes

- ✓ Footnotes may be used to provide pertinent information, but should be used sparingly.
- ✓ Use the following notations (etc.) instead of adding footnotes
  (xx%) by NMR, (xx%) by GC, (xx%) crude
- ✓ Write footnotes as short phrases, without a beginning capital letter or final period.
- ✓ Place footnotes in the entry (instead of at the end of the Table), and restart with ^{a} for each entry.

TABLE 5. CATALYTIC ENANTIOSELECTIVE IODOCYCLIZATION (*Continued*)

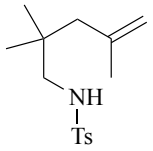
E. SULFONAMIDE *N*-NUCLEOPHILES

	Substrate	Conditions	Product(s) and Yield(s)	Refs.

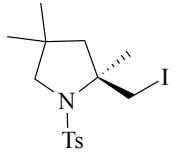
*Please refer to the charts preceding the tables for the structures indicated by the **bold** numbers.*

Tab05E-e004

C_8



L4 (0.25 eq), $Cu(OTf)_2$ (0.2 eq), *i*-PrI (5.9 eq), MnO_2 (3 eq), K_2CO_3, 4 Å MS, $PhCF_3$, 105 °C, 11 h

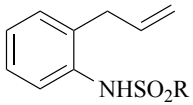


(74%) by GC, er = 58.0:42.0

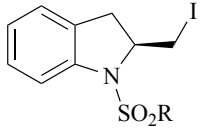
{Bovino, 2012 #112}

Tab05E-e005

C_9



Ligand (*x* eq), $Cu(OTf)_2$ (*y* eq), *i*-PrI (6 eq), MnO_2 (3 eq), K_2CO_3, 4 Å MS, $PhCF_3$, 105 °C, 6 h

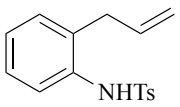


R	Ligand	*x*	*y*	Yield (%)	er	
Me	**L4**	0.25	0.2	85	90.5:9.5	
$Me_3Si(CH_2)_2$	**L4**	0.25	0.2	85	91.0:9.0	{Bovino,
4-BrC_6H_4	**L3**	0.25	0.4	77	94.0:6.0	2012
4-$O_2NC_6H_4$	**L4**	0.50	0.2	72	90.0:10.0	#112}
3,5-*t*-$Bu_2C_6H_3$	**L3**	0.25	0.2	90	—[a]	

[a] not separable by HPLC on a chiral stationary phase

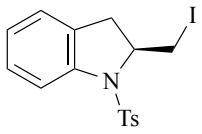
Tab05E-e006

C_9



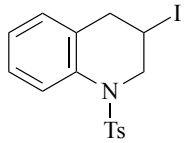
F1 (0.1 eq),[a] NIS (1.2 eq), KBr (0.02 eq), CH_2Cl_2, –78 ºC

[a] catalyst **F1** must be freshly prepared



(58%) er = 93.5:6.5

+



(14%)

{Mizar, 2014 #57}

APPENDIX I: Checklist for *Organic Reactions* Chapter Authors and Responsible Editors

The following requirements should be satisfied prior to submitting the final version of an Organic Reactions chapter to the Editorial Coordinator. Items on this list should serve as an interim checklist for a chapter in progress.

Item No.	Checked Item	Author's Initials	RespEd's Initials
1	**Before sending the manuscript for review by BOE members:**		
1a	EndNote is used for reference citations.		
1b	Each text graphic has a citation of only the reference from which the example is taken. If more references are relevant to the statement, the remaining citations are placed at the end of the sentence.		
1c	The text graphics illustrate the accompanying text, and any data provided with the graphic is in agreement with that presented in the text.		
1d	Reaction conditions include all reagents, equivalents, solvent, temperature, and time.		
1e	Depictions of stereochemical configurations follow OR format, as described in the MS Guide. All available (diastereomeric, enantiomeric, regioisomeric, etc.) ratios are reported.		
1f	Bold compound numbers in reaction graphics are used only to facilitate text discussions, and therefore must appear in the text if assigned to a structure. The only exceptions are catalyst/ligand numbers and numbers used in sub-tables for the purpose of combined yields and product ratios. Catalyst/ligand numbers are differentiated from the other numbered compounds in the text graphics.		
1g	The Experimental Procedures are well chosen to show the breadth of conditions used for the title reaction. The ordering matches the Scope and Limitations section, and a description of the reaction sub-type is [in square brackets] next to the product name. If available, a large-scale reaction is included. Analytical data for the product is carefully transcribed.		
	The manuscript has been reviewed by the appointed members of the Editorial Board, and the author has satisfactorily incorporated suggestions and made any necessary corrections.		

Item No.	Checked Item	Author's Initials	RespEd's Initials
2	**Before sending the completed Tables to the Editorial Coordinator for review:**		
2a	Entries appear in the correct table according to reaction type.		
2b	Within each Table, the entries are organized as described in the rubric that was approved at the chapter outline stage. Sub-table entries are organized by the same rubric.		
2c	Entries illustrating the same reaction on related substrates are either grouped in sub-tables or juxtaposed by elimination of protecting groups (or other non-critical substituents such as simple alkyl groups on heteroatoms, alkoxy group of esters, etc.) from the carbon count.		
2d	Reaction data include all reagents, equivalents, solvent, temperature, time, yield, and dr/er (if applicable).		
2e	The references are in the form of EndNote temporary citations; e.g., {Smith, 2021 #113}		
2f	The Tabular Survey Introduction (the last section of the text): 1. states whether the Tables include all the examples found in the literature, or are selective examples 2. states whether or not reactions shown in the text section of the chapter are repeated in the Tables 3. explains the ordering rubric		

Item No.	Checked Item	Author's Initials	RespEd's Initials
3	**To submit the chapter for final processing, include the following:**		
3a	Abstract (~250 words) and (10) Key Words as an MS Word document; add a shortened title to be used as running header (60 characters maximum, including spaces) if applicable.		
3b	Chapter Text, with embedded text graphics, in both MS Word and pdf formats.		
3c	EndNote library (A single EndNote library should be submitted for the entire chapter, and the record numbers must match those in the temporary citations in the Table files; e.g., {Smith 2021, #113})		
3d	ChemDraw files for text graphics (i.e., Schemes and Figures)		
3e	ChemDraw Tabular Survey files (i.e., Tables)		

APPENDIX II: Placement and Identification of Text Graphics

The following pages illustrate (1) a ChemDraw file containing text graphics to be submitted for processing; (2) a sample text page illustrating how the version is to look with the insertion numbers and associated graphics embedded for review by the Responsible Editor.

ChemDraw Files with Insertion Numbers and Titles

3

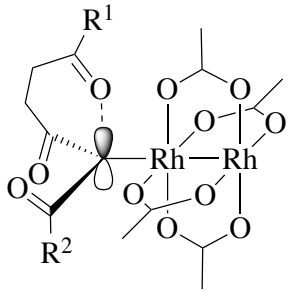
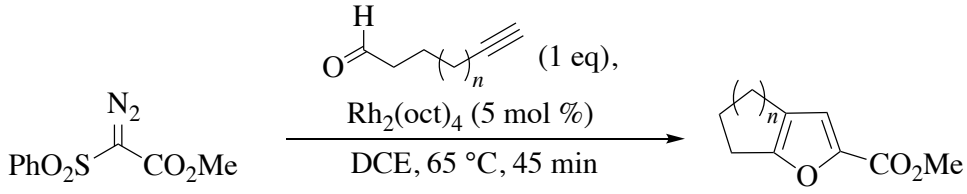


Figure 1. Possible transition state for formation of a metal-complexed cyclic ylide.

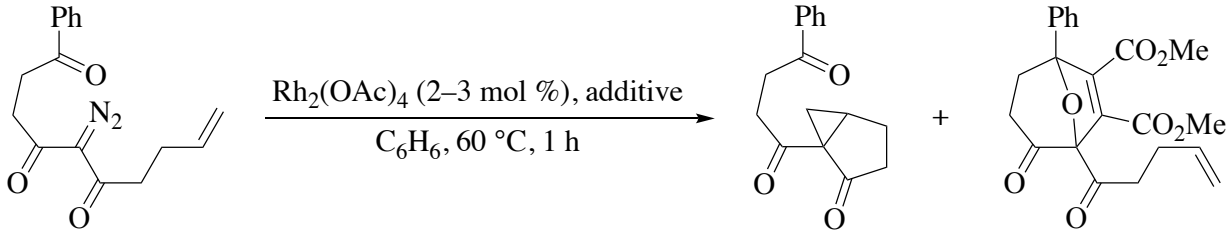
4



n	Yield (%)
1	46
2	65

Scheme 3

5



Additive		
—	81	—
DMAD (1.1 eq)	15	68

Scheme 4

This latter work suggests that a transition structure for cyclization to form a metal-complexed ylide might resemble that illustrated in Fig. 1, shown as derived from a 2-diazo-1,3,6-tricarbonyl substrate.

(3)

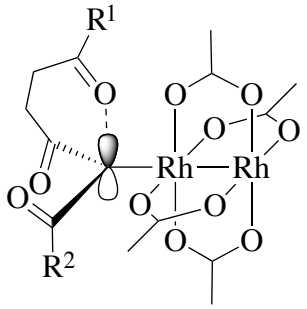
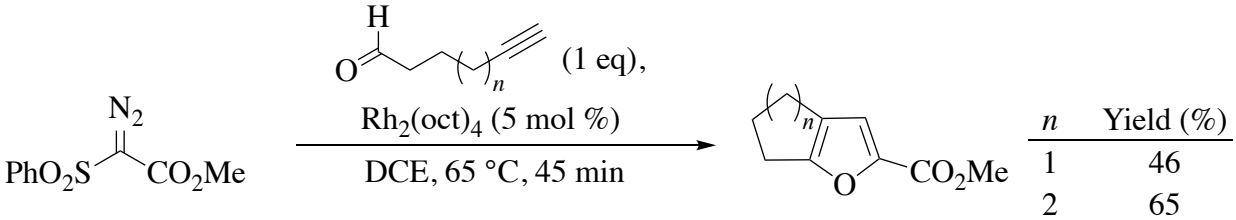


Figure 1. Possible transition state for formation of a metal-complexed cyclic ylide.

Experimental support for reversible ylide formation is found for reaction of a diazosulfone with two unsaturated aldehydes that compete for the diazosulfone in intermolecular carbonyl ylide formation–intramolecular cycloaddition.{Jones, 2012 #818} When used separately, 5-hexynal and 6-heptynal both undergo cycloaddition followed by elimination of benzenesulfinic acid, leading to a furan fused to either a five- or six-membered ring, respectively (Scheme 3).{Jones, 2012 #818}

(4)



n	Yield (%)
1	46
2	65

Scheme 3

APPENDIX III: Guidelines for Computer-Drawn Text Graphics

ChemDraw files for the text graphics must be submitted with the manuscript. Points of insertion for the graphics should be noted in the text just above the graphic itself (see APPENDIX II: Placement and Identification of Text Graphics).

A ChemDraw stationery file (*OR TxGr Stationery.cds*) is provided via e-mail. This file should be used as the style template for drawing text graphics.

To view the document settings, go to the "File" menu and select "Document Settings…"

Text graphics should be constructed with the page setup as “US Letter” in "portrait" mode.

Although the "Drawing" settings are the same as those required for the tables, the "Captions" and "Atom Labels" settings differ. Use 12-pt Times New Roman in both the "Captions" and "Atom Labels" settings; use fixed 16-pt line-spacing for captions, and fixed 10-pt line-spacing for atom labels.

APPENDIX III (*continued*)

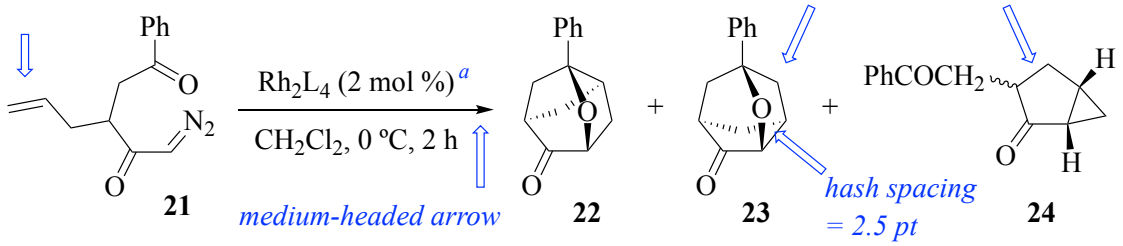
Annotated Example of a Text Graphic

Note: The ChemDraw stationery file, OR TxGr Stationery.cds, has all the correct settings.

Text settings (all)
font = Times New Roman
size = 12 pt
line spacing = 16 pt

bond length = 16.2 pt
line width = 0.5 pt

bond spacing = 2.92 pt



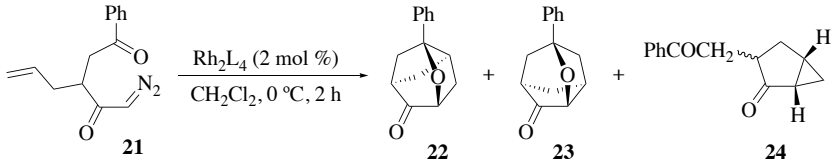
Catalyst	**22**–**24** Yield (%)	**22**/**23**/**24**
$Rh_2(OAc)_4$	94	11:50:39
$Rh_2(cap)_4$	96	13:54:33
$Rh_2(pfb)_4$	87	38:14:48
$Rh_2(tfa)_4$	93	37:13:50

Scheme 5

Preferred maximum 7" (17.8 cm/500 pt)
Absolute maximum 7.25" (18.4 cm/522 pt)

[a] For two-line conditions, use a single text box with 20-pt line spacing and center it over the arrow.

When processed by our publisher, the scheme printed in the actual volume at 67% reduction will look like this:



Catalyst	**22**–**24** Yield (%)	**22**/**23**/**24**
$Rh_2(OAc)_4$	94	11:50:39
$Rh_2(cap)_4$	96	13:54:33
$Rh_2(pfb)_4$	87	38:14:48
$Rh_2(tfa)_4$	93	37:13:50

Scheme 5

APPENDIX IV: Guidelines for Computer-Drawn Tables and Sub-Tables

Authors are referred to the website organicreactions.org to download instructional videos about preparing table files.

A ChemDraw stationery file (*OR Table Stationery.cds*) is provided via e-mail. This file should be used as the style template for drawing table entries.

To view the document settings, go to the "File" menu and select "Document Settings…"

Tables are prepared using US Letter size pages in landscape orientation. Note that "Pages" *NOT* "Poster" is selected in the Layout tab. The multi-page feature is *NOT* an option for the preparation of *Organic Reactions* Tables.

Although the "Drawing" settings are the same as those required for text graphics, the "Captions" and "Atom Labels" settings differ. Use 10-pt Times New Roman in both the "Captions" and "Atom Labels" settings; use fixed 16-pt line-spacing for captions, and fixed 9-pt line-spacing for atom labels.

Sample Table Files

The following two pages show how a finished page of table entries should appear. The first page shows a set of table entries, and the second shows the same set of entries plus an insertion, should adding an entry be necessary.

Sample File 1

TABLE 6. CROSS-COUPLING OF ARYL DIAZONIUM SALTS

	Redox Partner	Transition Metal Partner	Conditions	Product(s) and Yield(s)	Refs.

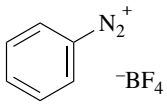
Notation indicates that this record is the 1st entry in Table 6.

These column widths may be adjusted as necessary, but must remain constant throughout a given Table, e.g., Table 6.

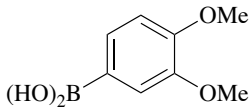
Alignment of Refs within the column will be adjusted when the final numbers are entered.

Tab06-e001

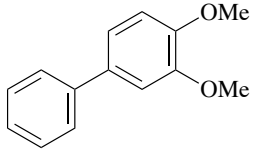
C_{12}



2.0 eq



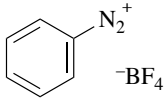
$Ru(bpy)_3(PF_6)_2$ (2.5 mol %),
$Au(PPh_3)NTf_2$ (5 mol %), H_2O (60 eq),
MeCN, CFL (20 W), rt, 16 h



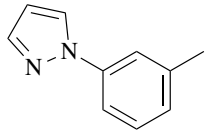
(83%) {Smith, 2013 #203}

Tab06-e002

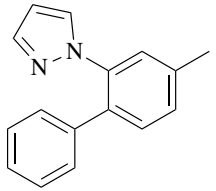
C_{13}



4.0 eq



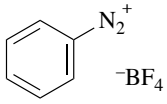
$Ru(bpy)_3Cl_2 \cdot 6H_2O$ (2.5 mol %),
$Pd(OAc)_2$ (10 mol %), Ag_2CO_3 (1.0 eq),
MeOH, CFL (26 W), 25 °C, 5 h



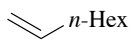
(53%) {Jones, 2014 #194}

Tab06-e003

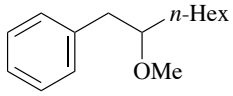
C_{14}



4.0 eq



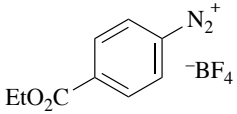
Fluorescein (5 mol %),
MeOH, CFL (23 W), –20 °C, 16 h



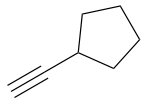
(86%) {Gupta, 2010 #210}

Tab06-e004

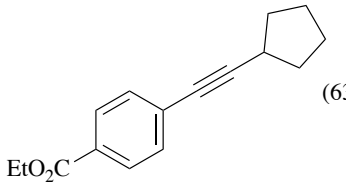
C_{14}



4.0 eq



$Ru(bpy)_3(PF_6)_2$ (0.5 mol %),
$Au[P(4\text{-}MeOC_6H_4)_3]Cl$ (10 mol %),
DMF, CFL (23 W), rt, 1 h



(63%) {Xi, 2009 #201}

Filename has the form AuthTab06-e001-, e.g. MacTab06-e001-.

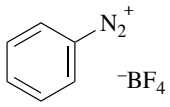
TABLE 6. CROSS-COUPLING OF ARYL DIAZONIUM SALTS

	Redox Partner	Transition Metal Partner	Conditions	Product(s) and Yield(s)	Refs.

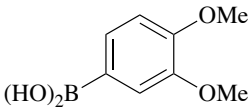
This file is a revision of the previous page, illustrating how to handle insertion/deletion.

Tab06-e001

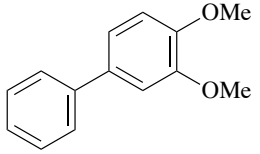
C_{12}



2.0 eq



$Ru(bpy)_3(PF_6)_2$ (2.5 mol %),
$Au(PPh_3)NTf_2$ (5 mol %), H_2O (60 eq),
MeCN, CFL (20 W), rt, 16 h

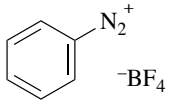


(83%) {Smith, 2013 #203}

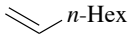
Tab06-e002-deleted ← *Make a note that the entry has been deleted.*

Tab06-e003

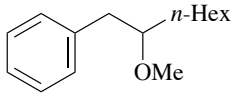
C_{14}



4.0 eq



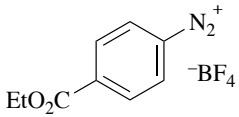
Fluorescein (5 mol %),
MeOH, CFL (23 W), –20 °C, 16 h



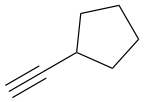
(86%) {Gupta, 2010 #210}

Tab06-e004

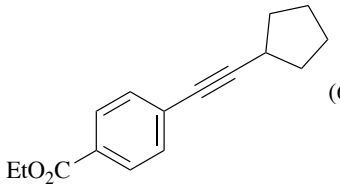
C_{14}



4.0 eq



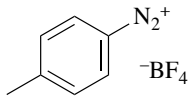
$Ru(bpy)_3(PF_6)_2$ (0.5 mol %),
$Au[P(4\text{-}MeOC_6H_4)_3]Cl$ (10 mol %),
DMF, CFL (23 W), rt, 1 h



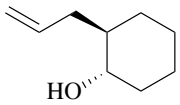
(63%) {Xi, 2009 #201}

Tab06-e004a ← *Use alpha-numeric notation to insert a new entry into a previously completed table to avoid re-numbering subsequent entries.*

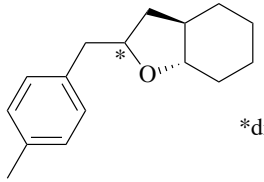
C_{16}



4.0 eq



$Ru(bpy)_3(PF_6)_2$ (2.5 mol %),
$Au(PPh_3)NTf_2$ (10 mol %),
MeOH, CFL (23 W), rt, 4–16 h



(66%) {Martin, 2001 #35}
*dr = 2.8:1.0

APPENDIX IV (*continued*)

How to Prepare the ChemDraw Table Files

The following is a transcription of the instructions given in the PowerPoint tutorial found on the *Organic Reactions Wiki Home Page* at http://organicreactions.org/index.php/Author_Center.

- **Create a stationery file for each separate Table** using the *OR Table Stationery.cds* file provided by the Editorial Coordinator as a template. Give each Table a number and a title. Number Tables using Arabic numerals. The first letter of each word in the title is in 12-pt (except for prepositions and conjunctions), and the remaining letters in 10-pt, all CAPS. Subdivisions, if used, should be numbered 2A, 2B, etc. The column headers may remain the same as in the generic stationery file, except the substrate column should be more descriptive if possible, e.g., amine, keto ester, etc. Center the column headings. Adjust column widths to best suit the anticipated entries, but leave both the guide-marks on the ends and the reference column guide-mark fixed. *Once column widths are set, they must remain constant throughout a given Table.*
- Select "Save as…" from the file menu to **save the file as a new stationery file** (.cds not .cdx). Once this new stationery file is opened it will become the default new document. Use this stationery file for every page of entries in that particular Table for which it was designed. Create a new stationery file with an appropriate header when beginning each new Table.
- **Construct and label table entries.** Open a stationery file as created above. Draw structures and type conditions and references for each table entry. (The proper drawing, atom label, and caption settings are part of the document settings in *OR Table Stationery.cds*, and will be in any new stationery file created from using this file as a template unless actively changed.) When a structure contains more than one object, e.g., brackets, parentheses, stereochemical notations, footnote letters, etc., group them together using "Group" in the "Object" menu. This step will ensure that the structure stays intact during subsequent alignment procedures. *Otherwise, do not group entries*.
- **Arrange entries within each Table in order of increasing carbon number** of the starting material. The carbon count should be based on all the carbon atoms that define the substrate minus carbons in standard protecting groups not involved in the reaction. Simple alkyl and aryl groups on oxygen and nitrogen should also be eliminated from the count, as it allows for the grouping of reactions that together demonstrate the effects of simple structural variations on the outcome of a reaction. Place C_5, C_6, etc. slightly above the entry and align with the left-most header guide-mark. If a set of similar substrates is grouped in one entry by using a sub-table, show the count as a range, for example $C_{5–11}$. Put such an entry in the carbon count group of the lower end of the range, in this example the C_5 group.
- **Repeat carbon counts, starting materials, and products for each entry.**

- **Include only 3 or 4 entries per page**, and separate them with a dotted line. (Leave extra space on the page in case insertion of an additional entry is necessary later.) Label each entry as to its Table and order in which it is to appear. For example, Tab01e004 indicates that the entry should be the fourth one in Table 1. Make every effort to have the order as close as possible to the final order.
- After all the entries are made, **align the contents of each column** using the "left edges" alignment tool in the "Object" pull down menu. *The contents of each column are left-aligned with the left-most guide-mark of that column.* Then align each entry using "T/B centers". Use 16-pt line spacing in all text boxes.
- **Name the file.** Name each file so that it is identifiable by author, table number, and insertion numbers: DenTab01e121– denotes that this file has entries starting from 121 for Table 1 in the Denmark chapter.
- To insert additional entries at a later time, either insert it into the proper file, or, if it will not fit, simply create a new page for the additional entry, and name it alphanumerically. An insertion code of Tab01e004a would put the entry between Tab01e004 and Tab01e005. (See sample files in this Appendix.)

Construction of Sub-Tables

As directed on page 28, sub-tables should be limited to those examples where the substrates and/or products are simple analogs, where the substrate and product(s) remain the same but conditions differ, or where simple analogs are subjected to slightly different conditions. Details are provided below.

- ✓ Sub-tables in Table entries should be ordered by the same logic used for ordering of the table entries, e.g., by increasing carbon count. Text graphics sub-table entries may be ordered to match the order of discussion in the associated text.
- ✓ Each type of data should have its own column, e.g., er values should not be included in the same text box as the yield.
- ✓ For categories like "catalyst" or "additive", include the term in the conditions, and then provide the specifics in the sub-table. Use a variable for the eq if it is not the same in every example [e.g., additive (*x* eq)], and then include a column for that variable.
- ✓ Create one column at a time. Include the column header (R, Temp (°C), etc.) in the same text box.
- ✓ Use 16-pt line-spacing.
- ✓ Left-align text.
- ✓ Center numerical data such as yield, temperature, and time. For sub-tables in the Tables and text graphics, the "Yield (%)" sub-header is used and no parentheses are used around the yield.
- ✓ Select all the columns in the sub-table, and use the "align top edges" and then the "distribute horizontally" commands (found under the "Objects" menu in ChemDraw).

- ✓ Add a line (from the brackets icon in the drawing tools) under the column headings, then group ("Objects" menu).
- ✓ In both Tables and text graphics, if there are different references in a sub-table, enter them in the reference column in the same rows as the entries to which they refer.
- ✓ Scale partial structures in sub-tables by 85%, keeping the atom labels the original font size.
- ✓ If some of the data points do not apply to all the entries in the sub-table, use the following notations:

  yield: — for yield not reported; 0 for none formed
  solvent: — for not reported; neat for none used
  all other cases (cat., stoich, temp, time, etc.): — for not used or not reported

- ✓ Orientations of Substituent Abbreviations in Sub-Tables:

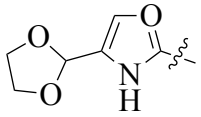
Me	MeO_2S	H_2N	Ph
CF_3	CF_3CO	O_2N	Py
HCO	AcO	NC–	1-Np
t-Bu	$AcOCH_2$	CN–	3-MeC_6H_4
n-C_5H_{11}	EtO_2C	MeO	3-$MeOC_6H_4$
c-C_6H_{11}	4-$TolSO_3$	BnO	2,5-$(MeO)_2C_6H_3$

✓ General Appearance of Properly Constructed Sub-Tables

In Table Entries (organized by carbon count)

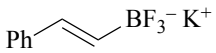
				Yield (%)		
R^1	R^2	Temp (°C)	Time (h)	**I** + **II**	**I/II**	
MeO_2S	Me	35	3	96	2.7:1	{Hong, 2004 #952}
MeO_2C	Me	80	1	89	4.2:1	{Takahashi, 2003 #960}
MeO_2S	Ph	101	24	68	—	{Korotchenko, 2004 #942}
MeO_2S	Ph	101	24	82	6.3:1	{Aames, 2010 #839}

In Text Graphics (organized by order of text discussion or by carbon count)

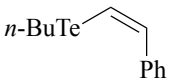
			Yield (%)		
R	Temp (ºC)	Time (h)	**6** + **7**	**6**/**7**	Refs
MeO_2C	25	4.7	60	5.8:1	{Raju, 2006 #63}
$BnO(CH_2)_2$	25	3	75	9.1:1	{Raju, 2006 #63}
allyl	25	3	70	3.0:1	{Raju, 2006 #63}
	80	3	65	15:1	{Nakadaira, 1972 #195}
(*E*)-PhCH=CH	80	4.5	66	10:1	{Nakadaira, 1972 #195}

Example 1: Table Entry Sub-Table of Different Conditions

C_8

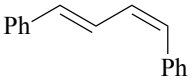


"single isomer"



"single isomer"

$Pd(PPh_3)_4$ (20 mol %),
base (2 eq), additive (2 eq),
MeOH, ultrasound, 23 ºC, 20 min



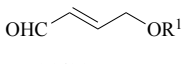
"single isomer"

{Wicha, 2004 #951}

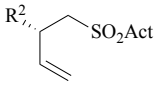
Base	Additive	Yield (%)
K_2CO_3	Ag_2O	65
Cs_2CO_3	Ag_2O	67
Et_3N	Ag_2O	66
Et_3N	AgOAc	84

Example 2: Table Entry Wherein Substrates/Products Are Simple Analogs and Conditions Differ

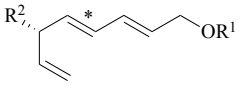
C_4



(*E*)/(*Z*) = 99:1



1. $MN(SiMe_3)_2$ (1.2 eq), solvent, –78 °C, 30 min
2. Aldehyde (*x* eq); then to rt, 1 h

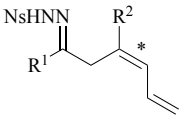


R^1	R^2	Act	M	Solvent	*x*	Yield (%)	$^*(E)/(Z)$	
PMB	Me	PT	Li	DME	1.0	71	84:16	{Gaertner, 2013 #1891}
TBDPS	Me	BT	Li	DME	1.1	88	88:12	{Gaertner, 2013 #1891}
PMB	Et	PT	K	THF	1.5	58	69:31	{Ulver, 2006 #503}

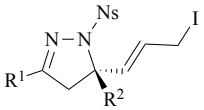
---

example from a different Table:

$C_{13–22}$



C10 (0.1 eq), NIS (1.2 eq), toluene/CH_2Cl_2 (3:1), 4 Å MS, –80 °C, 72 h



{Tripathi, 2015 #43}

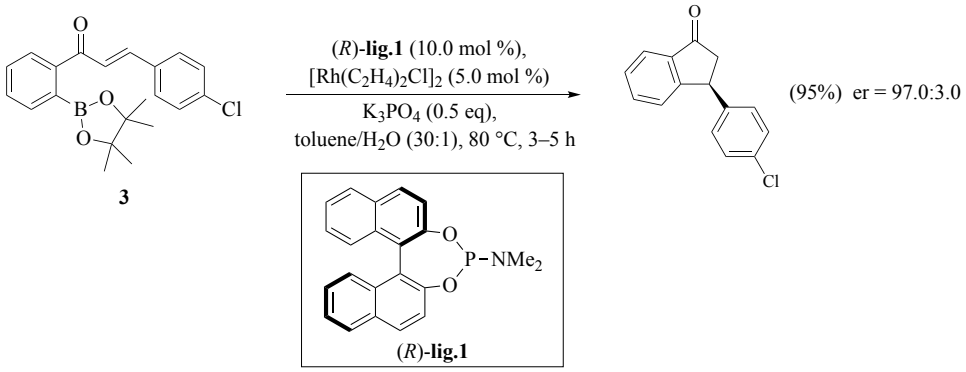
*Config	R^1	R^2	Yield (%)	er
(*Z*)	*c*-C_6H_{11}	Me	43	67.0:33.0
(*E*)	*c*-C_6H_{11}	Ph	66	95.0:5.0
(*E*)	Ph	Me	61	96.5:3.5

APPENDIX V: Ligand/Catalyst Numbering

- Use the same number for both enantiomers of a ligand/catalyst.
- Include the absolute stereochemistry [i.e., (*R*)- or (*S*)-] with the number; if the structure has >2 stereocenters, "**L1**" and "*ent*-**L1**" (for example) may be used instead.

Text Graphics:

- ✓ The ligands/catalysts are numbered by order of appearance in the text graphics.
- ✓ Use "**lig.x**" and "**cat.x**" to distinguish the numbered ligands/catalysts from the other numbered compounds in the text graphics.
- ✓ The numbers for each ligand/catalyst **will not match** between the text graphics and the Tables.
- ✓ The ligand/catalyst structure should be drawn in the first text graphic in which it is used, underneath the reaction, in a box. After the first occurrence, only the number should be used. *Exception: the ligands should be redrawn for every Experimental Procedure graphic.*

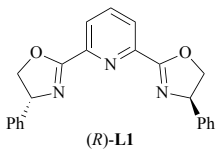


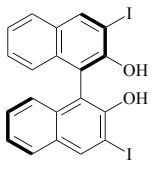
Scheme 10

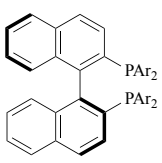
Tables:

- ✓ Use a ligand chart and a catalyst chart, and any additional charts as necessary (e.g., amine chart, acylating agent chart, etc.). Note that each Chart should contain the specified structures for the entire Tabular Survey; do not prepare a separate Chart for each Table.
- ✓ The ligands/catalysts are generally numbered by order of appearance in the Tables, continuously from Table 1 to Table x. Subtables may be used for similar structures.
- ✓ Use the notation **Lx** and **Cx**.
- ✓ The ligand/catalyst structure should not be drawn in the first table entry in which it is used.

CHART 1. LIGANDS USED IN THE TABLES





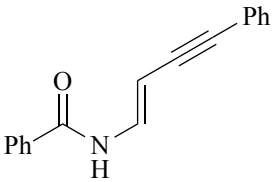


Ligand	Ar
(*S*)-**L3**	3,5-*i*-$Pr_2C_6H_3$
(*S*)-**L4**	Ph
(*S*)-**L5**	3,5-$Me_2C_6H_3$
(*S*)-**L6**	4-MeC_6H_4

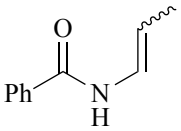
APPENDIX VI: Guidelines for Stereochemical Depictions

*Refer to page 22 for additional information. Note that the same rules listed here for product structures also apply to **starting material** structures.*

- Double bond specifications: draw the major isomer with a straight bond when the (*E*)/(*Z*) ratio is known; use a wavy bond if the ratio is unknown.



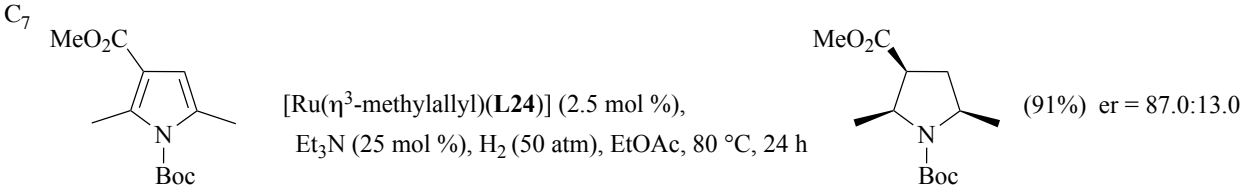
(85%) (*E*)/(*Z*) = 2:1



(75%)

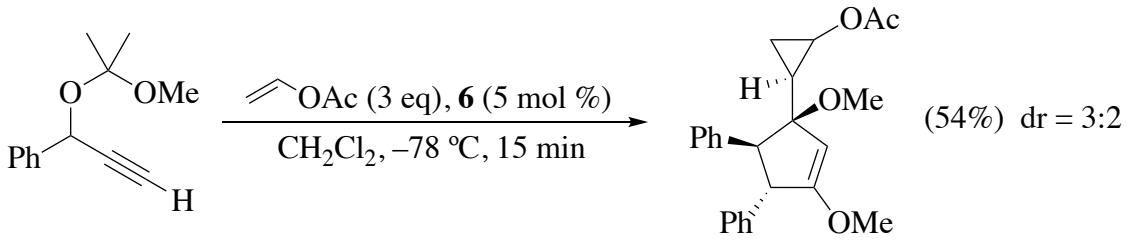
- Draw the major isomer when the product is a mixture of isomers with specified composition and known configuration. Structures of minor isomers may be included if necessary for clarity.

Example Table Entry



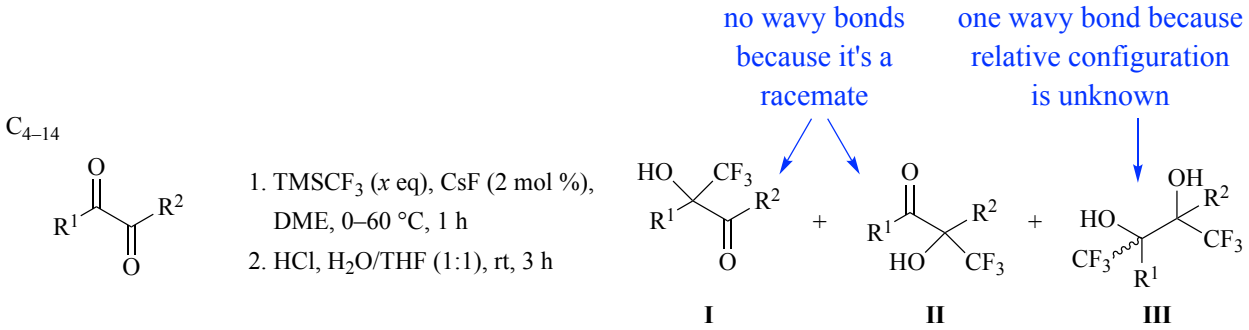
- Use a straight line for the key bond when the product is a single isomer or a mixture of isomers with specified composition, but no configurational assignment. A single structure denoting a racemic mixture should also use straight-line bonds.

Example Text Graphic



- Use a wavy line for the key bond when the product is a mixture of unknown composition.

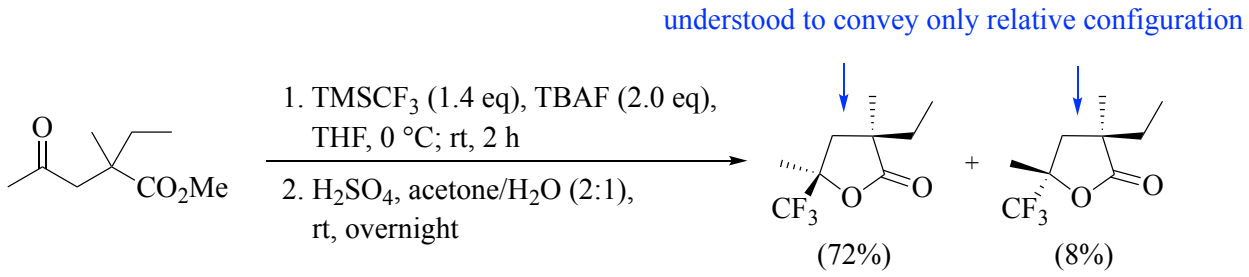
Example Table Entry



			Yield (%)		
R^1	R^2	*x*	**I** + **II**	**I**/**II**	Yield (%) **III**
Me	Me	3	—	—	78
Ph	Ph	2.25	94	—	—

- Relative stereochemistry can be shown on diastereomeric products from a racemic starting material.

Example Text Graphic

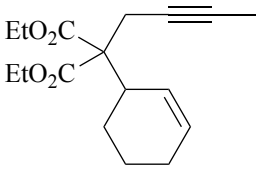


- Report **all available ratios** for regioisomers, diastereomers, and enantiomers in the text graphics and table entries. The dr/er/(*E*)-(*Z*) ratios for <u>starting materials</u> should also be included if the ratios can be affected by the reaction.

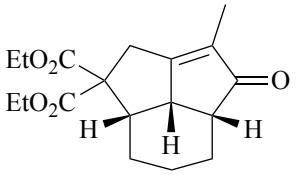
- If needed for clarity, statements such as the following can be added below structures:

  major diastereomer
  configuration unspecified
  "single enantiomer", "single diastereomer" (with quotation marks)
  - See "Reporting Regioisomeric and Stereochemical Ratios" section for specific rules for using these terms.

C_{13}



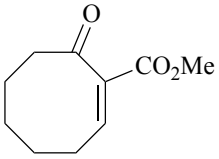
C6 (10 mol %),
CO (0.34 atm),
toluene, 90 ºC



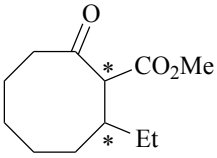
(86%)

"single diastereomer"

C_9



(*S*,*S*)-**OP186** (10 mol %),
$Cu(OTf)_2$ (10 mol %),
$ZnEt_2$ (3 mol %),
CH_2Cl_2, 23 ºC, 17 h



(65%) er = 99.0:1.0

* rel and abs config undetermined

APPENDIX VII: Styles for Selected Abbreviations and Symbols

USE	*INSTEAD OF*
Me, Et	CH_3,CH_3CH_2
i-Pr, *t*-Bu	$(CH_3)_2CH$, $(CH_3)_3C$, ^{i}Pr, ^{t}Bu
n-C_6H_{13}	$CH_3(CH_2)_5$
4-MeC_6H_4, 3-Cl-4-MeC_6H_3	*p*-MePh, *m*-Cl-*p*-MeC_6H_3

Abbreviations for cyclic substituents:		*Use the following forms:*
cyclopentyl	*c*-C_5H_9	4 Å MS
cyclohexyl	*c*-C_6H_{11} or Cy	2 N HCl
naphthyl	1-Np or 2-Np	0.5 M HCl (in MeOH)
pyridyl	Py	Na_2SO_4•$10H_2O$
tolyl	Tol	aq NaOH
		mol %
		*h*ν

SHORTCUTS FOR COMMONLY USED SYMBOLS AND SIGNS

Symbol	Mac Shortcut	PC Shortcut*	Example
º	shift-option-8 or option-0	Alt-0176	23 °C
•	option-8	Alt-0149	BF_3•OEt_2
-	hyphen		*N*-acetyl, *t*-Bu
–	option-hyphen	Alt-0150	–78 °C, 32–54%
—	shift-option-hyphen	Alt-0151	(—)
α	Symbol font a		α-keto ester
β	Symbol font b		β-keto ester
ν	Symbol font n		*h*ν
Å	shift-option-a	Alt-0197	4 Å MS
±	shift-option-=	Alt-0177	± 95%
≥	option-.	Alt-242	er ≥ 99.9%
≤	option-,	Alt-243	≤ 7%
×	Symbol font option-e	Alt-0215	3 × 25 mL
→	Symbol font option-r		*N*→*O* acyl shift

*with numlock on in Word, but off in Chemdraw

APPENDIX VIII: *The Journal of Organic Chemistry* Standard Abbreviations and Acronyms

Available as a pdf file from the *Journal of Organic Chemistry*:
http://pubs.acs.org/userimages/ContentEditor/1218717864819/joceah_abbreviations.pdf

α	observed optical rotation in degrees
[α]	specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]
Å	angstrom(s)
Ac	acetyl
acac	acetylacetonate
ADP	adenosine 5'-diphosphate
AIBN	2,2'-azobisisobutyronitrile
AMP	adenosine 5'-monophosphate
Anal.	combustion elemental analysis
anhyd	anhydrous
AO	atomic orbital
aq	aqueous
Ar	aryl
atm	atmosphere(s)
ATP	adenosine 5'-triphosphate
ATPase	adenosinetriphosphatase
av	average
9-BBN	9-borabicyclo[3.3.1]nonyl
9-BBN–H	9-borabicyclo[3.3.1]nonane
BINOL	1,1'-bi-2-naphthol
Bn	benzyl
BOC, Boc	*tert*-butoxycarbonyl
BODIPY	dipyrromethene boron difluoride
bp	boiling point, base pair
bpy	2,2'-bipyridyl
br	broad (spectral)
Bu, *n*-Bu	normal (primary) butyl
s-Bu	*sec*-butyl
t-Bu	*tert*-butyl
Bz	benzoyl (not benzyl)
B3LYP	3-parameter hybrid Becke exchange/Lee–Yang–Parr correlation functional
°C	degrees Celsius
calcd	calculated
cAMP	adenosine cyclic 3',5'-phosphate
CAN	ceric ammonium nitrate
CASSCF	complete active space self-consistent field
CASPT2	complete active space with second-order perturbation theory
cat	catalytic
CBZ, Cbz	benzyloxycarbonyl (preferred over the abbreviation Z)
CC	coupled cluster
CD	circular dichroism
cDNA	complementary deoxyribonucleic acid
CI	chemical ionization; configuration interaction
CIDNP	chemically induced dynamic nuclear polarization
CIF	Crystallographic Information Framework
cm	centimeter(s)
cm^{-1}	wavenumber(s)
compd	compound
concd	concentrated
concn	concentration
COSY	correlation spectroscopy
Cp	cyclopentadienyl
m-CPBA	*meta*-chloroperoxybenzoic acid
CV	cyclic voltammetry
Cy	cyclohexyl
δ	chemical shift in parts per million downfield from tetramethylsilane
d	day(s); doublet (spectral); deci
d	density
DABCO	1,4-diazabicyclo[2.2.2]octane
dansyl	5-(dimethylamino)-1-naphthalenesulfonyl
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DCC	*N,N*'-dicyclohexylcarbodiimide
DCE	1,2-dichloroethane
DCM	dichloromethane
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DEAD	diethyl azodicarboxylate
DEPT	distortionless enhancement by polarization transfer
DFT	density functional theory
DIBALH	diisobutylaluminum hydride
DMA	dimethylacetamide
DMAP	4-(*N,N*-dimethylamino)pyridine
DMDO	dimethyldioxirane
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
DMSO	dimethyl sulfoxide
DMT	4,4'-dimethoxytrityl (4,4'-

	dimethoxyltriphenylmethyl)
DNA	deoxyribonucleic acid
DPS	*tert*-butyldiphenylsilyl
dr	diastereomer ratio
DTT	dithiothreitol
E1	unimolecular elimination
E2	bimolecular elimination
EA	ethyl acetate
ED_{50}	dose effective in 50% of test subjects
EDTA	ethylenediaminetetraacetic acid
EI	electron impact
EPR	electron paramagnetic resonance
eq	equation
equiv	equivalent
er	enantiomer ratio
ESI	electrospray ionization
Et	ethyl
FAB	fast atom bombardment
FD	field desorption
FID	flame ionization detector; free induction decay
Fmoc	9-fluorenylmethoxycarbonyl
FT	Fourier transform
g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g. gCOSY, gHMQC)
GC	gas chromatography
GTP	guanosine 5'-triphosphate
h	hour(s)
HF	Hartree–Fock
HMBC	heteronuclear multiple bond correlation
HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
HMQC	heteronuclear multiple quantum correlation
HOMO	highest occupied molecular orbital
HPLC	high-performance liquid chromatography
HRMS	high-resolution mass spectrometry
HSQC	heteronuclear single quantum correlation
Hz	hertz
ICR	ion cyclotron resonance
IP	ionization potential
IR	infrared
IRC	intrinsic reaction coordinate
J	coupling constant (in NMR spectrometry)
k	kilo
K	kelvin(s) (absolute temperature)
L	liter(s)
LAH	lithium aluminum hydride
LCAO	linear combination of atomic orbitals
LD_{50}	dose that is lethal in 50% of test subjects
LDA	lithium diisopropylamide; local density approximation
LFER	linear free energy relationship
LHMDS	lithium hexamethyldisilazane, lithium bis(trimethylsilyl)amide
lit.	literature value (abbreviation used with period)
LTMP	lithium 2,2,6,6-tetramethylpiperidide
LUMO	lowest unoccupied molecular orbital
μ	micro
m	multiplet (spectral); meter(s); milli
M	molar (moles per liter); mega
M^+	parent molecular ion
MALDI	matrix-assisted laser desorption ionization
max	maximum
MCD	magnetic circular dichroism
MCR	multicomponent reaction
MCSCF	multi-configuration self-consistent field
MD	molecular dynamics
Me	methyl
MEM	(2-methoxyethoxy)methyl
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl (mesyl)]
MHz	megahertz
min	minute(s); minimum
mM	millimolar (millimoles per liter)
MM	molecular mechanics/modeling
MO	molecular orbital
mol	mole(s); molecular (as in mol wt)
MOM	methoxymethyl
mp	melting point
MRCI	multi-reference configuration interaction
mRNA	messenger ribonucleic acid
Ms	methylsulfonyl (mesyl)
MS	mass spectrometry
MTBE	methyl *tert*-butyl ether
MW, mol wt	molecular weight
m/*z*	mass-to-charge ratio (not *m*/*e*)
N	normal (equivalents per liter)
NAD^+	nicotinamide adenine dinucleotide
NADH	reduced NAD
NBO	natural bond orbital
NBS	*N*-bromosuccinimide
NCS	*N*-chlorosuccinimide
NHC	N-heterocyclic carbene
NICS	nucleus-independent chemical shift
NIS	*N*-iodosuccinimide
nm	nanometer(s)
NMO	*N*-methylmorpholine-*N*-oxide
NMP	*N*-methylpyrrolidone

NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NOESY	nuclear Overhauser effect spectroscopy
NRT	natural resonance theory
Nu	nucleophile
OD	optical density
ORD	optical rotary dispersion
PCC	pyridinium chlorochromate
PDC	pyridinium dichromate
PE	petroleum ether
PES	photoelectron spectroscopy
Ph	phenyl
piv	pivaloyl
pm	picometer(s)
PMB	*p*-methoxybenzyl
PPA	poly(phosphoric acid)
ppm	part(s) per million
Pr	propyl
*i*Pr	isopropyl
PTC	phase-transfer catalysis
py	pyridine
q	quartet (spectral)
QM	quantum mechanics
QSAR	quantitative structure–activity relationship
RCM	ring-closure metathesis
redox	reduction–oxidation
rel	relative
R_f	retention factor (in chromatography)
RHF	restricted Hartree–Fock
ROESY	rotating frame Overhauser effect spectroscopy
ROMP	ring-opening metathesis polymerization
rRNA	ribosomal ribonucleic acid
rt	room temperature
s	singlet (spectral); second(s)
SAR	structure–activity relationship
SCF	self-consistent field
SEM	scanning electron microscopy; 2-trimethylsilylethoxymethyl
SET	single electron transfer
S_N1	unimolecular nucleophilic substitution
S_N2	bimolecular nucleophilic substitution
S_N'	nucleophilic substitution with allylic rearrangement
SOMO	single-occupied molecular orbital
t	triplet (spectral)
t	time; temperature in units of degrees Celsius (ºC)
T	absolute temperature in units of kelvins (K)
TBAB	tetrabutylammonium bromide
TBAC	tetrabutylammonium chloride
TBAF	tetrabutylammonium fluoride
TBS	*tert*-butyldimethylsilyl
TBHP	*tert*-butyl hydroperoxide
TCA	trichloroacetic acid
TCNE	tetracyanoethylene
TDDFT	time-dependent density functional theory
TEAB	tetraethylammonium bromide temp temperature
TEMPO	2,2,6,6-tetramethylpiperidin-1-oxyl
TES	triethylsilyl
Tf	trifluoromethanesulfonyl (triflyl)
TFA	trifluoroacetic acid
TFAA	trifluoroacetic anhydride
THF	tetrahydrofuran
THP	tetrahydropyran-2-yl
TIPS	triisopropylsilyl
TLC	thin-layer chromatography
TMAI	tetramethylammonium iodide
TMEDA	*N,N,N',N'*-tetramethyl-1,2-ethylenediamine
TMS	trimethylsilyl; tetramethylsilane
TOF	time-of-flight; turnover frequency
TON	turnover number
Tr	triphenylmethyl (trityl)
tRNA	transfer ribonucleic acid
t_R	retention time (in chromatography)
Ts	*para*-toluenesulfonyl (tosyl)
TS	transition state
UHF	unrestricted Hartree–Fock
UV	ultraviolet
VCD	vibrational circular dichroism
vis	visible
vol	volume
v/v	volume per unit volume (volume-to-volume ratio)
wt	weight
w/w	weight per unit weight (weight-to-weight ratio

APPENDIX IX: Chart for Converting % ee into er

% ee	er	% ee	er	% ee	er
1	50.5:49.5	34	67.0:33.0	67	83.5:16.5
2	51.0:49.0	35	67.5:32.5	68	84.0:16.0
3	51.5:48.5	36	68.0:32.0	69	84.5:15.5
4	52.0:48.0	37	68.5:31.5	70	85.0:15.0
5	52.5:47.5	38	69.0:31.0	71	85.5:14.5
6	53.0:47.0	39	69.5:30.5	72	86.0:14.0
7	53.5:46.5	40	70.0:30.0	73	86.5:13.5
8	54.0:46.0	41	70.5:29.5	74	87.0:13.0
9	54.5:45.5	42	71.0:29.0	75	87.5:12.5
10	55.0:45.0	43	71.5:28.5	76	88.0:12.0
11	55.5:44.5	44	72.0:28.0	77	88.5:11.5
12	56.0:44.0	45	72.5:27.5	78	89.0:11.0
13	56.5:43.5	46	73.0:27.0	79	89.5:10.5
14	57.0:43.0	47	73.5:26.5	80	90.0:10.0
15	57.5:42.5	48	74.0:26.0	81	90.5:9.5
16	58.0:42.0	49	74.5:25.5	82	91.0:9.0
17	58.5:41.5	50	75.0:25.0	83	91.5:8.5
18	59.0:41.0	51	75.5:24.5	84	92.0:8.0
19	59.5:40.5	52	76.0:24.0	85	92.5:7.5
20	60.0:40.0	53	76.5:23.5	86	93.0:7.0
21	60.5:39.5	54	77.0:23.0	87	93.5:6.5
22	61.0:39.0	55	77.5:22.5	88	94.0:6.0
23	61.5:38.5	56	78.0:22.0	89	94.5:5.5
24	62.0:38.0	57	78.5:21.5	90	95.0:5.0
25	62.5:37.5	58	79.0:21.0	91	95.5:4.5
26	63.0:37.0	59	79.5:20.5	92	96.0:4.0
27	63.5:36.5	60	80.0:20.0	93	96.5:3.5
28	64.0:36.0	61	80.5:19.5	94	97.0:3.0
29	64.5:35.5	62	81.0:19.0	95	97.5:2.5
30	65.0:35.0	63	81.5:18.5	96	98.0:2.0
31	65.5:34.5	64	82.0:18.0	97	98.5:1.5
32	66.0:34.0	65	82.5:17.5	98	99.0:1.0
33	66.5:33.5	66	83.0:17.0	99	99.5:0.5

er = [(100+%ee)/2]: [(100–%ee)/2]

APPENDIX X: Copy Editing and Proofreading Symbols

Mark	Meaning	Marked in Proof	Corrected
—	Set in italics (ital)	Goethe's Faust	Goethe's *Faust*
~~	Set in boldface (bf)	*J. Org. Chem.* 1993	*J. Org. Chem.* **1993**
rom	Set in roman (rom)	prepared *in situ*	prepared in situ
≈	Set in small capitals (sc)	D-glucose	D-glucose
≡	Set in capitals (cap)	new york	New York
lc	Set in lowercase (lc)	in Benzene	in benzene
[	Move left	[where t = time	where *t* = time
]	Move right	(25a)]	(25a)
tr	Transpose	of teh ester	of the ester
¶	Paragraph indent	¶ Carbodesilylation is an	Carbodesilylation is an
tr ↓	Transfer down	alternative to lateral lithiat-	alternative to lateral lithia-
⌒	Run in	ion methodology. ⌒ Fluoride-induced	tion methodology. Fluoride-induced coupling of....
⌴	Move down	x^{y}	xy
⌐	Move up	x_{y}	xy
^	Set as subscript	xy	x_y
v	Set as superscript	xy	x^y
#	Insert space	isan alternative to	is an alternative to
⌐	Delete	right-hand hand page	right-hand page
⌐	Delete and close up	right-hand page	right-hand page
=	Set hyphen	high frequency radiation	high-frequency radiation
⌐	Delete hyphen, close up	sub topic	subtopic
⌐	Delete hyphen, leave space	cross section	cross section
⊙	Set a period	J. Am Chem. Soc.	*J. Am. Chem. Soc.*
^,	Set a comma	1993 108 56	**1993**, *108*, 56
^:	Set a colon	been prepared azaindole	been prepared: azaindole
^;	Set a semicolon	one-pot process however	one-pot process; however
↓	Set a prime	2-methyl-4-cyano-	2-methyl-4'-cyano-
stet	Ignore correction		