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# *ORGANIC REACTIONS*

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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*. Templates and samples are available in the Author Center of our website: **organicreactions.org**. For the chapter text, we rely primarily on the guidelines provided in *The ACS Style Guide*,<sup>†</sup> 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.

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 is a publication of consistently high quality that continues to serve as a principal reference series. We are grateful to our authors, who help to maintain the high caliber of *Organic Reactions*.

*The Editorial Board of Organic Reactions*

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

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# QUICK START: CHAPTER PREPARATION IN A NUTSHELL

## Tools Provided

(available in the Author Center at [organicreactions.org](http://organicreactions.org))

- *Organic Reactions Manuscript Guide* (illustrates all the necessary style and formatting details)
- *Templates*
- *Samples*: outline, table organization rubric, text, text graphics, tables and charts, abstract
- *Videos on table file preparation* ([organicreactions.org](http://organicreactions.org))

## General Description of Steps

1. Attend Zoom meeting with Responsible Editor and Editorial Coordinator.
2. Review the MS Guide, and consult the Format Checklist in Appendix I to better understand the requirements for the final product.
3. Collect references into EndNote.
4. Submit for review:
  - ✓ **Outline** of entire chapter, with complete listing of tables.  
[This resembles the Table of Contents, but with additional explanation where needed.]
  - ✓ **Table Organization Rubric**  
[This will become the Tabular Survey Introduction in the chapter.]

**Do not proceed to samples until the Outline and Rubric have been approved!**

5. Submit for review:
  - ✓ **Text sample**: 10 p from Mechanism & Stereochemistry + 10 p from Scope & Limitations
  - ✓ **Text Graphics sample**: the ChemDraw files for the inserts in the text samples
  - ✓ **Table samples**: A) 5 filled ChemDraw files from each of two different tables (“TS-I”); *then*  
B) 2 entire tables (“TS-II”, incorporating changes from “TS-I”)

**Do not proceed with chapter preparation until samples have been approved!**

6. Stay in contact with your Responsible Editor (every 3 months at a minimum) as you write the chapter. Follow the prompts in the Text Template for each text section. For the Tabular Survey, choose examples that best illustrate the scope of the reaction, and order the entries as defined in the approved rubric.
7. Note that chapters undergo several successive reviews by multiple editors. Consult the Chapter Steps Checklist (link emailed by the Editorial Coordinator at chapter initiation) to see which steps have been completed.

## Final Submission Components

1. Abstract, Key Words, Running Header (MS Word) and Graphical Abstract (ChemDraw)
2. Manuscript (MS Word and PDF)
3. Text Graphics (ChemDraw)
4. Tabular Survey (ChemDraw)
5. References (EndNote library)
6. Completed Format Checklist

## REQUIREMENTS FOR FINAL CHAPTER 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, Keywords, Graphical Abstract, Running Header.** The online version of an *Organic Reactions* chapter includes an abstract. The author should submit 10 keywords and a 300-word abstract as a Microsoft (MS) Word file to the Responsible Editor with the final copy of the chapter. The abstract should be a concise description of the materials in the article and its implications, and should include all keywords. Do not include references to other articles, or URLs.

A graphical abstract will be used to advertise the chapter on [organicreactions.org](http://organicreactions.org). The graphical abstract must be no larger than 6 inches wide x 2 inches tall (15 cm x 5 cm). Color should be used judiciously.

A shortened title to be used as running header should be submitted by the author if the chapter title exceeds 60 characters, including spaces.

**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 multipage 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 galley proofs 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 based on the collaboration 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). The Editorial Coordinator provides the author with this MS Guide, templates for each chapter section, and links to the Format Checklist and Chapter Steps Checklist. Subsequently, the Editorial Coordinator and Responsible Editor have a Zoom meeting with the author and co-authors to explain *Organic Reactions* formats and procedures.

Authors must submit to the Responsible Editor a detailed proposed Outline of the chapter, divided by chapter sections, and with a complete list of 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.* Approval of the Outline and Rubric typically requires several rounds of reviews.

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. Approval of the samples typically requires several rounds of reviews. 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 Introduction (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 tables for adherence to guidelines and accuracy of organization before arranging for vetting, as noted below.

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

Ultimately, 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 Responsible Editor 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 in the Author Center at [organicreactions.org](http://organicreactions.org).

- ✓ 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.

## ***Text Sections***

### **Title Page**

Include:

- ✓ Chapter Title
- ✓ Authors' full names
- ✓ 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**

### **TABLE OF CONTENTS**

Include:

- ✓ 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.

The Table of  
Contents should  
match the actual  
text headings  
and  
subheadings.

### **ACKNOWLEDGMENTS**

*(Optional)*

Be concise!

## INTRODUCTION

- ✓ 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*

## 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.
- ✓ Illustrate the origin of selectivity with schemes and/or figures.

## 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.)*

- ✓ This section should mirror the organization of the Tabular Survey. Exceptions should be approved by the Editor-in-Chief.
- ✓ 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.

Double-check  
for faithful  
transcription  
of information.

- ✓ Do not present full optimization studies; instead, focus on the optimized reaction conditions.
- ✓ 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 (with ratio if a mixture of 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. Place the citation at the end of the sentence that refers to the scheme/figure.
- ✓ Include *current* limitations on the scope of the reaction.
- ✓ Suggest new applications or extensions of the reaction.



#### COMMON ERRORS

*Discussion lacks critical commentary.*

*Excessive number of reaction examples.*

*Reaction graphic conditions are incomplete.*

*Reaction graphics are inaccurate.*

*Reaction graphics do not illustrate associated text.*

*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 methods to form the same products as obtained by the title reaction, detailing the advantages and disadvantages of each method.
- ✓ In addition to substrate and product structures, the depicted reactions must include all reagents and their stoichiometric amounts, solvents (with ratio if mixture of solvents), temperature, time, isolated yield, and regioisomeric and stereochemical ratios.
- ✓ If possible, cross-reference with specific examples in Scope and Limitations for comparison.

## EXPERIMENTAL CONDITIONS

- ✓ Identify significant hazards and safety precautions. Set warnings in italics, beginning 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

- ✓ Each procedure title should include the product name, and in square brackets a description of the reaction subtype.
- ✓ Include several different procedures to illustrate significant variations and applications of the reaction, being careful to minimize repetition.
- ✓ Choose examples that provide the most detailed description of the experiment, with stoichiometry of all reactants and reagents, isolated yields, purification methods, and **full characterization** of the products ( $^1\text{H}$ - and  $^{13}\text{C}$ -NMR, IR, MS, etc.). For enantioselective/enantiospecific reactions, the method used to determine enantiomeric ratio should be included (e.g., column, eluant, rate and retention times). An experimentalist should be able to reproduce the reaction and identify the products using only the procedure in the *Organic Reactions* chapter.
- ✓ When molar equivalents are not available (such as in enzyme-catalyzed reactions), report quantities as published in the primary literature (e.g., g enzyme/mol SM).

- ✓ Include a large-scale preparation if available in the literature, particularly any industrial application on kilogram scale.



#### 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 text, text graphics, and tables 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 INTRODUCTION

- Note that Table divisions should be based on substrate (or product) structures, NOT on catalyst/ligand used.
- Approval must be obtained from the Editor-in-Chief if the Tabular Survey is organized differently than the Scope and Limitations section.

- ✓ Provide the cutoff date for the literature survey.
- ✓ State whether or not the tables include all the examples in the literature, or only selective examples.
- ✓ State whether or not the reactions in the text graphics (Schemes) are repeated in the tables. *Note that either all or none of the in-text reactions (except those in the Comparison with Other Methods section) should be repeated in the tables.*
- ✓ Explain the use of charts, if any.
- ✓ Describe the organization of the Tabular Survey:
  - 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 any unusual conventions used in the Tabular Survey.

## ***General Format and Style of the Manuscript Text***

### **Text Section Headers**

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 subheadings in the text agree with those listed in the Table of 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...

## Text Style and Format

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. American spelling should be used in the chapter.

The following *Organic Reactions* rules are different than those 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."

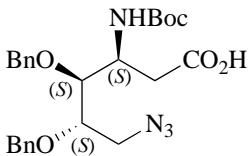
- ✓ (*R*), (*S*), (*Z*), and (*E*) are *always italicized and in parentheses*. The parentheses themselves, however, are not italicized.

(*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 (%)	( <i>E</i> )/( <i>Z</i> )	Catalyst	Yield (%)	er
	Me	13	2:1	( <i>R,S</i> )- <b>C3</b>	76	95.0:5.0
	<i>i</i> -Pr	49	4:1	( <i>S,S</i> )- <b>C14</b>	55	99.5:0.5
	Ph	41	1:2			

- ✓ 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 instead of formulas for chemicals in the text. However, formulas of complex chemicals can be used instead of their names; i.e.,  $\text{LiAlH}(\text{O}t\text{-Bu})_3$  vs. lithium tri(*tert*-butoxy)aluminum hydride.
- ✓ A trivial name or acronym can be used if a common chemical with a long name is mentioned repeatedly. Define the acronym at the first point of use in the text and in the List of Abbreviations.
- ✓ 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.”
- ✓ In general, use brackets to denote cycloadditions; e.g., [4+2]. Use parentheses if the number of electrons participating in the cycloaddition is different than the number of participating atoms; e.g., (4+3). Do not use a space before or after the + sign.
- ✓ *Use the passive voice in present or past tense throughout the text, but use only the past tense for the Experimental Procedures.*

### ***Specific Conventions for Experimental Procedures***

- ✓ Illustrate the procedure with a reaction graphic. Type in the insertion number and insert the graphic, both above the procedure.
- ✓ Follow the name of the product with a short phrase identifying the reaction type:  

**Methyl 3-Amino-2-thioformylcrotonate [Thioformylation of an Enamine].**<sup>30</sup> A solution of  $\text{POCl}_3$  (0.5 mL, 5.5 mmol) 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  $\text{Et}_2\text{O}$ ,  $\text{EtOAc}$ , THF, DMF, DMSO,  $\text{CH}_2\text{Cl}_2$ ,  $\text{CHCl}_3$ , 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;  $^1\text{H}$  NMR;  $^{13}\text{C}$  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 °C, 5 °C/min, then 100 to 180 °C, 0.5 °C/min, 15 psi)
- ✓  $[\alpha]_D^{25} + 85.0$  (*c* 0.02, MeOH)
- ✓ UV (hexanes)  $\lambda_{\max}$  ( $\epsilon$ ): 250 (1070)
- ✓ FTIR (NaCl) 1824, 1454, 1248, 1102, 942  $\text{cm}^{-1}$
- ✓  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.30–7.10 (m, 5H), 5.29 (dd,  $J = 6.4, 8.5$  Hz, 1H), 5.13 (d,  $J = 14.9$  Hz, 1H)
  - shifts to 2 decimal places and coupling constants to 1 decimal place
- ✓  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  174.3, 135.4, 128.7
  - shifts to one decimal place
  - duplicate shifts marked with (2C)
- ✓ LRMS–CI ( $\text{NH}_3$ ) ( $m/z$ ):  $[\text{M} + \text{H}]^+$  423, 367, 349
- ✓ HRMS–ESI ( $m/z$ ):  $[\text{M} + \text{Na}]^+$  calcd for  $\text{C}_{13}\text{H}_{16}\text{O}_2\text{Na}$ , 227.1048; found, 227.1046.
  - formula should be of the detected compound; e.g., include Na if detected as the Na salt
- ✓ Anal. Calcd for  $\text{C}_{18}\text{H}_{15}\text{F}_3\text{O}_2$ : 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 insertion 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);<sup>53</sup> the reaction is selective for vinylogous amides with aryl alkynes, and is selective for lactams when alkyl alkynes are used.<sup>53,54</sup>”
- ✓ If a scheme has reactions from more than 1 reference, the associated text or the scheme should clarify which reference each reaction is from (e.g., a Refs column in a subtable).
- ✓ Schemes and figures should be placed after the paragraph describing them. Multiple schemes can be inserted after a paragraph.
- ✓ 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 (in Word file): Scheme 1 / Fig. 1  
graphics (in ChemDraw file): **Scheme 1** / **Figure 1**. Legend.

- ✓ 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 in the ChemDraw files and/or are not included in the text.*

*"Schemes" are labeled as "Equations".*

*Figures do not include legends.*

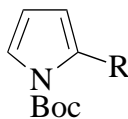
*Text graphic Scheme/Figure labels are in the Word file instead of the ChemDraw file.*

## Numbering Structures

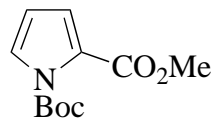
If the discussion requires reference to a structure in a text graphic, identify the structure with a **boldface** Arabic numeral and use the same boldface numeral in the text. Structure numbers should be assigned in numerical sequence in order of appearance in the text graphics, beginning with the number **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 use Roman Numerals in the text graphics.
- ✓ Do not use the same Arabic number for a general structure and a specific structure. For example:



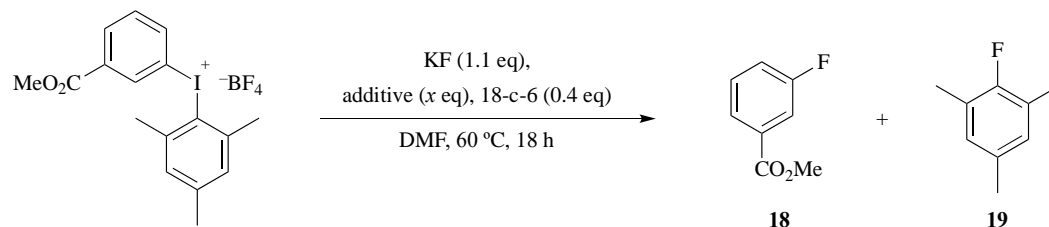
**7**



**8**

- ✓ *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 subtable ratios and yields.



Additive	x	Yield (%)		Refs
		<b>18 + 19</b>	<b>18/19</b>	
—	—	64	50:50	{Cabrele, 2016 #76}
Cu(OTf) <sub>2</sub>	0.2	73	94:6	{D'Auria, 2000 #17}
AlCl <sub>3</sub>	0.1	55	93:7	{Jones, 2018 #32}

- ✓ Note that ligands and catalysts will have different numbers in the text graphics versus in the tables. This allows authors to choose to prepare either the text or the tables first.
- ✓ See Appendix V for additional important instructions for ligand numbering.



#### COMMON ERRORS

Compound numbers are assigned to every structure, or are overused.  
Subtables 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 \$300 per chapter to offset the purchase of EndNote. This reimbursement will be made upon submission of a publishable chapter (steps 10D and 15 in the Chapter Steps Checklist). The receipt should be emailed to the *Organic Reactions* Treasurer.

### EndNote

- ✓ Database search results can be transferred directly into an EndNote library.
- ✓ Insert citations into the Text with the Cite While You Write function. Place reference citations in the text *after* any punctuation.
- ✓ To insert citations into the Table entries: select the reference in the EndNote library, and hit “copy” in the Edit menu; switch to the ChemDraw file, hit “paste” in the Edit menu.
- ✓ Note that EndNote cannot create a bibliography from .cdx files. Submit the table files with temporary citations (e.g., {Davis, 2012 #53}). *Organic Reactions* has a process for creating the bibliography from the temporary citations in the ChemDraw 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.

ChemDraw stationery files were provided at chapter initiation, and are available in the Author Center at [organicreactions.org](http://organicreactions.org). *Use these stationery files as templates for the preparation of text and table graphics.*

### USE THESE FILES!

OR TxGr Stationery.cds

OR Chart Template.cds

OR Graphical Abstract.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.

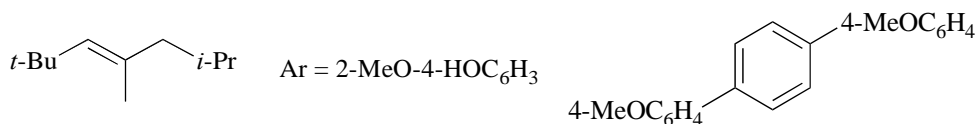
The following guidelines apply to formulas and structures in both text graphics and tables. When more than one style is acceptable, choose one and use it consistently throughout the chapter. Also see the sections “Specific Conventions for Text Graphics” and “Specific Conventions for Tables”.

See Appendix VII for preferred abbreviations and keyboard shortcuts for symbols

- ✓ Use abbreviations or acronyms for long chemical names in conditions. A list of approved abbreviations published by the *Journal of Organic Chemistry* is reproduced in Appendix VIII.
- ✓ Prepare a list of abbreviations/acronyms used in the chapter (text, text graphics, and tables) to be published at the end of the chapter. Only include the abbreviations/acronyms that do **not** appear in the JOC list.
- ✓ Number sequential steps using 1., 2., etc., not 1), 2), etc.
- ✓ In both the text graphics and the tables, *reaction details must include the stoichiometry of the reactants and reagents, solvent (with ratio if a mixture of solvents), 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 °C, 10 min.
- ✓ Use the following notation for solvent mixtures: MeCN/CH<sub>2</sub>Cl<sub>2</sub> (3:1).
- ✓ Use an en-dash for minus signs, optical rotation, and number ranges (e.g., temp, time, yields, carbon counts). The en-dash is formed with option-hyphen on a Mac, Alt-0150 on a PC; e.g., 10–23 °C.
- ✓ Do not use charge signs on simple salts. Use charge signs, not circled, on complex salts.
- ✓ To make charge signs, use the ChemDraw uncircled charge templates, or use superscripted + and en-dash.
- ✓ Use the ChemDraw radical dot for radicals.
- ✓ If carbon numbering is needed on a structure, use a font size 2 points smaller than the normal text.
- ✓ Use the 'open bond' to represent methyl attached to carbon.
- ✓ Use "Me" for methyl attached to a heteroatom.
- ✓ Use R<sup>1</sup>, R<sup>2</sup>, R<sup>3</sup>; not R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> or R, R', R''
- ✓ Use X only for a halogen, HX for a 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.



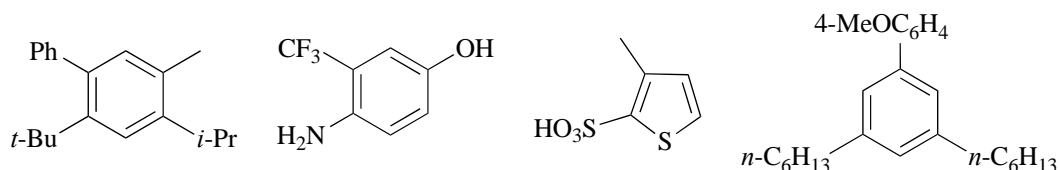
- ✓ Except for captions defining “R–” groups, use line drawings, not linear formulas.



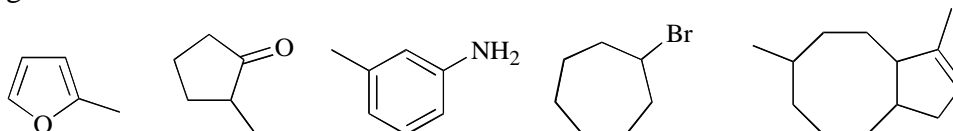
- ✓ Use Kekulé bonds in aromatic rings. The inscribed circle or ellipse should be used only for ions, complexes, and ferrocene-type compounds.
- ✓ Use the regular pentagon, not the "log cabin," for 5-membered rings.



- ✓ If it is necessary to save space or relieve crowding, formula designations for common cyclic and heterocyclic rings can be used.
- ✓ Draw hydrocarbon 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.

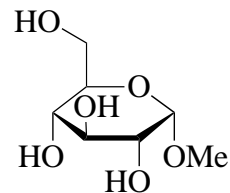
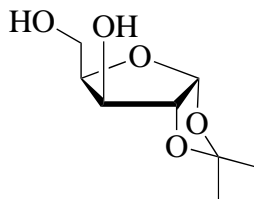
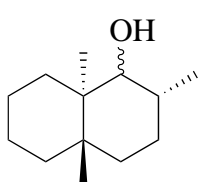
Orientation rules may be modified if the structure is complex, the rings are not involved in the chemical transformation, or orientation is dictated by a consistent representation of a reactant.

- ✓ 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% size (13.77 pt)** if the structure is 1) over a reaction arrow, 2) in the Conditions column of a table entry, 3) in a subtable, or 4) a partial structure to define an R group. **However, do not scale atom labels.**

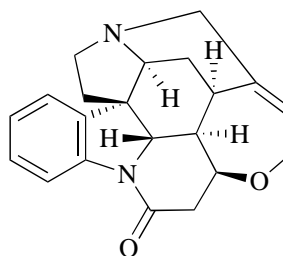
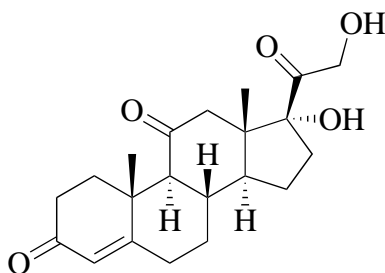
## Stereochemical Depiction

- ✓ 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.

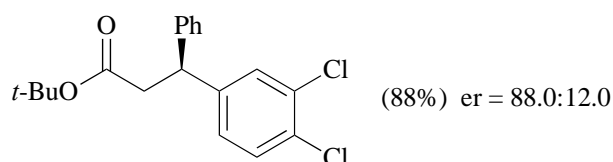


- ✓ See the next pages about the use of wedged/hashed bonds versus straight bonds versus wavy bonds, and reporting isomer ratios.

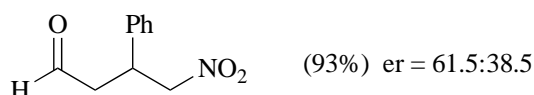
*Use the bonds as described below, whether or not they match the bond usage in the reference. Authors should determine the appropriate bond to use based on the data provided in the text and Supporting Information of the reference rather than reporting the depiction in the graphic of the reference.*

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

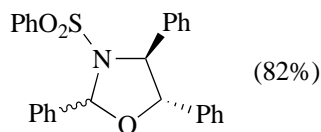
- Draw the major isomer when the product is a mixture of isomers with specified composition and known configuration. Structures of minor isomers may be included if necessary for clarity.



- 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.



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



✓ 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 <sup>1</sup>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.
- ✓ Color may be used in the schemes and figures.
- ✓ 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.
- ✓ Always use the medium-headed arrow, even for cyclic mechanisms.
- ✓ Do not use slanted arrows, and minimize the use of left-running arrows and vertical 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 17 for details about numbering.
- ✓ Limited subtables may be used to illustrate the scope of a reaction shown in a scheme. Consult Appendix IV for proper subtable format.
- ✓ Use “**lig.x**” and “**cat.x**” to distinguish the numbered ligands/catalysts from the other numbered compounds in the text graphics.
- ✓ 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 label “**lig.x**” or “**cat.x**” should be used. However, the ligands should be redrawn for every Experimental Procedure graphic. See Appendix V for complete instructions regarding catalysts and ligands.



### **COMMON ERRORS**

The small arrowhead is used.

Vertical, left-running, or slanted arrows are used unnecessarily.

### ***Specific Conventions for Table Graphics***

- ✓ Unlike the text graphics, the tables .cdx files should never be inserted into a Word file.
- ✓ Capitalize the first word in the Conditions column.
- ✓ 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.

$n\text{-C}_6\text{F}_{13}\text{I}$ (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 <sub>2</sub> SO <sub>4</sub> , H <sub>2</sub> O, rt, 5 min
---	---

- ✓ 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. Number the ligands with the notation **Lx** and catalysts with the notation **Cx**.
- ✓ The ligand/catalyst structure should not be drawn in the first table entry in which it is used. Instead, use the associated bold notations **Lx** and **Cx** in the table entries to refer readers to the structures in the charts. See **Appendix V** for complete instructions regarding catalysts and ligands.

# 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.*

- ✓ All examples from optimization studies should **NOT** be included. Instead, choose the best 1–3 conditions to exemplify the point of the study.
- ✓ In both the text graphics and the tables, *reaction details must include the stoichiometry of the reactants and reagents, solvent (with ratio if a mixture of solvents), temperature, time, yield, and isomeric ratios.* (Because these values are not always reported in the primary literature, make a note in the Tabular Survey Introduction 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.**



## ***Entry Ordering***

- ✓ 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.
- ✓ The table divisions should mirror the Scope and Limitations sections. Editor-in-Chief approval must be obtained if this is not the case.
- ✓ 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 (secondary ordering; e.g., oxidation state, ring size, etc.).
- ✓ 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).

**Recommended aryl group ordering within a carbon count**

1. Aryl group: *phenyl* > *naphthyl* > *anthracenyl* (etc.) > *heteroaryl* (by increasing atomic number)
2. Number of substituents: *unsubstituted* > *monosubstituted* > *disubstituted* > *trisubstituted*, etc.
3. Position of substituents: by increasing position number relative to reacting group
4. Identity of substituents: *H* > *halogen* (by increasing atomic number) > *heteroatoms* (by increasing atomic number) > *carbon*
5. Substrates that are otherwise identical: order by reacting group: *halogen* (by increasing atomic number) > *heteroatoms* (by increasing atomic number)

**Format**

Authors are referred to the Author Center on the *Organic Reactions* website, [organicreactions.org](http://organicreactions.org), to **view videos** on table and subtable preparation:

- ✓ Appendix IV has step-by-step instructions for table files preparation.
- ✓ **DO NOT use the multipage 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 subtable 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 45 in Appendix IV for suggested exclusions from the count.

### **Substrate/Starting Material**

- ✓ Include the structure for the starting material in every entry.
- ✓ Orient structures of starting materials and products similarly.
- ✓ If the substrate is not the limiting reagent, place the stoichiometry either centered under the structure or aligned at the same position throughout the table.

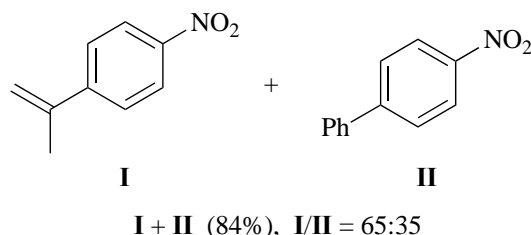
### **Conditions**

- ✓ Include the conditions for each entry, even if it repeats from the previous 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 subtable within an entry. Use the notation "(—)" for unreported yields and use (0%) if the product was not observed. Yield columns in subtables 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.



## References

- ✓ Use EndNote citations for table entries, as described earlier in the section beginning on page 19.
- ✓ 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 subtable is constructed from the same reference, use the reference number once, and align it with the structures. If different references contribute to the subtable, show each reference in the reference column in line with the corresponding subtable entry.

## Subtables

See  
Appendix IV for  
Tabular Survey  
subtable  
examples.

### ***Important Note on the Use of Subtables***

The use of subtables in individual table entries is recommended for analysis of the effects of simple structural changes or alteration of conditions on the outcome of a reaction. Subtables should be limited to those examples where the substrates and/or products are simple analogs, or where the structures are the same and conditions differ slightly (e.g., same reagents, but different catalysts, times, and/or temperatures).

**Complete instructions for constructing subtables are in Appendix IV.**

- ✓ Entries in subtables within table entries should be ordered by the same rubric as used for the table entries.

- ✓ In both the tables and text graphics, if a subtable contains entries from multiple references, add a reference column to the subtable.
- ✓ Substituent attachment points should be consistent within the subtable (MeO and MeO<sub>2</sub>C, or OMe and CO<sub>2</sub>Me, but not a mixture), except hydrocarbon substituents should always be written in direct form (e.g., *n*-C<sub>6</sub>H<sub>13</sub>).
- ✓ Use an en-dash to show the point of connection in potentially ambiguous R groups (NC–, CN–).

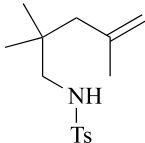
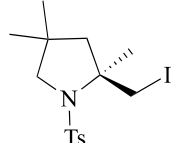
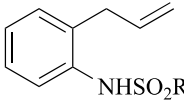
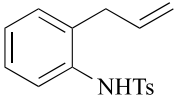
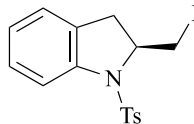
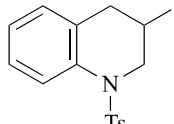
### ***Footnotes***

- ✓ 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, with a beginning capital letter and final period.
- ✓ Place footnotes in the entry (instead of at the end of the Table), and restart with <sup>a</sup> for each entry.

## Example Table File with Footnotes

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 <b>bold</b> numbers.																																								
<b>Tab05E-e004</b>																																								
C <sub>8</sub>		<b>L4</b> (0.25 eq), Cu(OTf) <sub>2</sub> (0.2 eq), <i>i</i> -PrI (5.9 eq), MnO <sub>2</sub> (3 eq), K <sub>2</sub> CO <sub>3</sub> , 4 Å MS, PhCF <sub>3</sub> , 105 °C, 11 h	 (74%) by GC, er = 58.0:42.0	{Bovino, 2012 #112}																																				
<hr/>																																								
<b>Tab05E-e005</b>																																								
C <sub>9</sub>		Ligand ( <i>x</i> eq), Cu(OTf) <sub>2</sub> ( <i>y</i> eq), <i>i</i> -PrI (6 eq), MnO <sub>2</sub> (3 eq), K <sub>2</sub> CO <sub>3</sub> , 4 Å MS, PhCF <sub>3</sub> , 105 °C, 6 h	<table><thead><tr><th>R</th><th>Ligand</th><th><i>x</i></th><th><i>y</i></th><th>Yield (%)</th><th>er</th></tr></thead><tbody><tr><td>Me</td><td><b>L4</b></td><td>0.25</td><td>0.2</td><td>85</td><td>90.5:9.5</td></tr><tr><td>Me<sub>3</sub>Si(CH<sub>2</sub>)<sub>2</sub></td><td><b>L4</b></td><td>0.25</td><td>0.2</td><td>85</td><td>91.0:9.0</td></tr><tr><td>4-BrC<sub>6</sub>H<sub>4</sub></td><td><b>L3</b></td><td>0.25</td><td>0.4</td><td>77</td><td>94.0:6.0</td></tr><tr><td>4-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub></td><td><b>L4</b></td><td>0.50</td><td>0.2</td><td>72</td><td>90.0:10.0</td></tr><tr><td>3,5-<i>t</i>-Bu<sub>2</sub>C<sub>6</sub>H<sub>3</sub></td><td><b>L3</b></td><td>0.25</td><td>0.2</td><td>90</td><td>—<sup>a</sup></td></tr></tbody></table>	R	Ligand	<i>x</i>	<i>y</i>	Yield (%)	er	Me	<b>L4</b>	0.25	0.2	85	90.5:9.5	Me <sub>3</sub> Si(CH <sub>2</sub> ) <sub>2</sub>	<b>L4</b>	0.25	0.2	85	91.0:9.0	4-BrC <sub>6</sub> H <sub>4</sub>	<b>L3</b>	0.25	0.4	77	94.0:6.0	4-O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	<b>L4</b>	0.50	0.2	72	90.0:10.0	3,5- <i>t</i> -Bu <sub>2</sub> C <sub>6</sub> H <sub>3</sub>	<b>L3</b>	0.25	0.2	90	— <sup>a</sup>	{Bovino, 2012 #112}
R	Ligand	<i>x</i>	<i>y</i>	Yield (%)	er																																			
Me	<b>L4</b>	0.25	0.2	85	90.5:9.5																																			
Me <sub>3</sub> Si(CH <sub>2</sub> ) <sub>2</sub>	<b>L4</b>	0.25	0.2	85	91.0:9.0																																			
4-BrC <sub>6</sub> H <sub>4</sub>	<b>L3</b>	0.25	0.4	77	94.0:6.0																																			
4-O <sub>2</sub> NC <sub>6</sub> H <sub>4</sub>	<b>L4</b>	0.50	0.2	72	90.0:10.0																																			
3,5- <i>t</i> -Bu <sub>2</sub> C <sub>6</sub> H <sub>3</sub>	<b>L3</b>	0.25	0.2	90	— <sup>a</sup>																																			
<sup>a</sup> Not separable by HPLC on a chiral stationary phase.																																								
<hr/>																																								
<b>Tab05E-e006</b>																																								
C <sub>9</sub>		<b>F1</b> (0.1 eq), <sup>a</sup> NIS (1.2 eq), KBr (0.02 eq), CH <sub>2</sub> Cl <sub>2</sub> , −78 °C	 +  (58%) er = 93.5:6.5      (14%)	{Mizar, 2014 #57}																																				
<sup>a</sup> Catalyst <b>F1</b> must be freshly prepared.																																								

## 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
<b>1</b>	<b>Before sending the manuscript for review by BOE members:</b>		
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 subtables 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 subtype 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.		
	<b>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.</b>		

Item No.	Checked Item	Author's Initials	RespEd's Initials
2	<b>Before sending the completed tables to the Editorial Coordinator for review:</b>		
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. <u>Subtable entries are organized by the same rubric.</u>		
2c	Entries illustrating the same reaction on related substrates are either grouped in subtables or juxtaposed by elimination of protecting groups (or other noncritical 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	<p>The Tabular Survey Introduction (the last section of the text):</p> <ol style="list-style-type: none"> <li>1. states whether the tables include all the examples found in the literature, or are selective examples</li> <li>2. states whether or not reactions shown in the text section of the chapter are repeated in the tables</li> <li>3. explains the ordering rubric</li> </ol>		



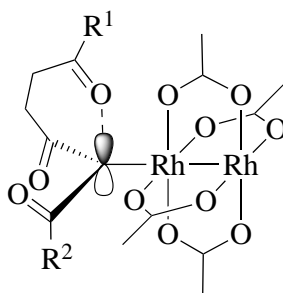
Item No.	Checked Item	Author's Initials	RespEd's Initials
<b>3</b>	<b>To submit the chapter for final processing, include the following:</b>		
3a	Abstract (~250 words) and (10) Key Words as an MS Word document; add a shortened title to be used as running header (60 characters maximum, including spaces) 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, <u>#113</u> })		
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.

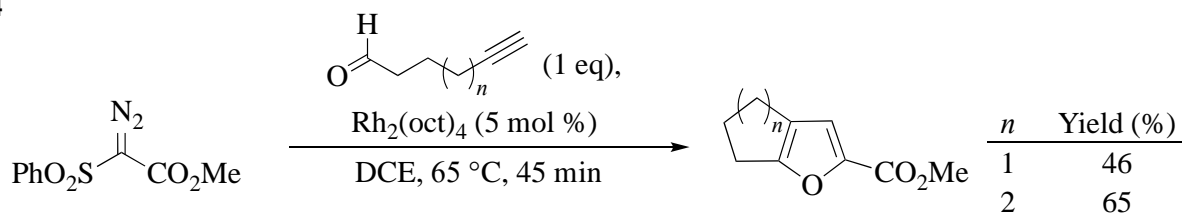
### *ChemDraw Files with Insertion Numbers and Titles*

3



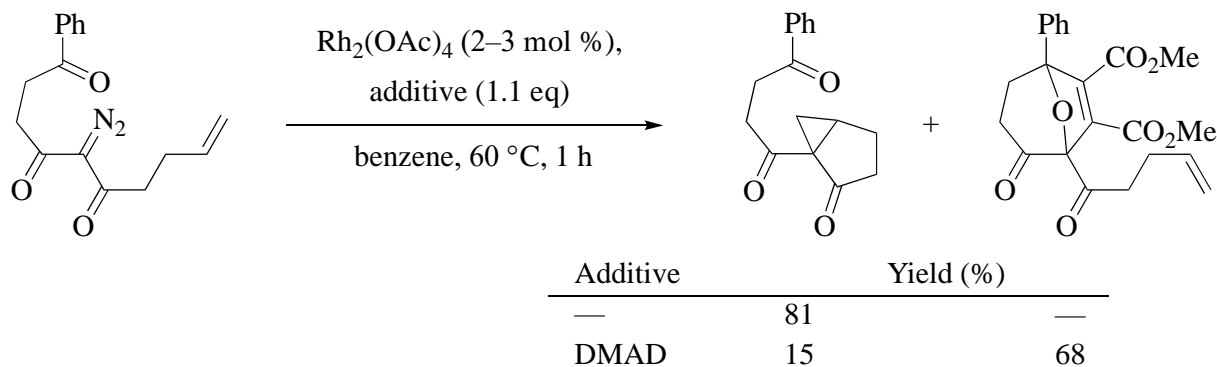
**Figure 1.** Possible transition state for formation of a metal-complexed cyclic ylide.

4



**Scheme 3**

5

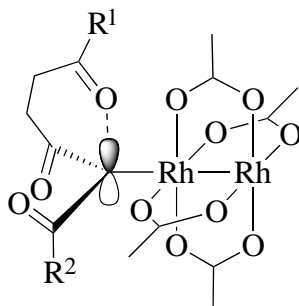


**Scheme 4**

## ***Sample Text with Insertion Numbers and Embedded Graphics***

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.

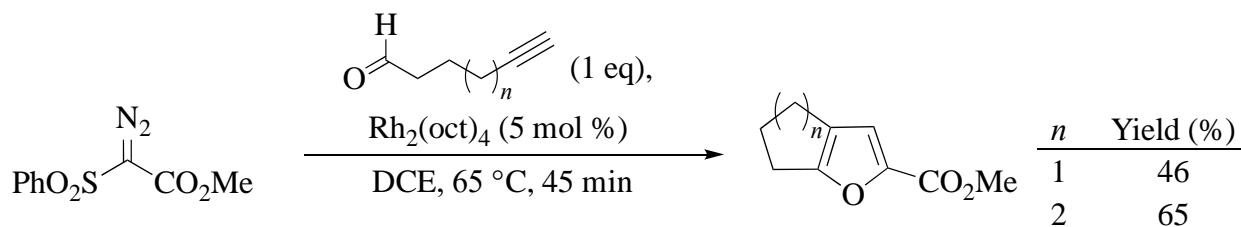
(3)



**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)



**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 and is available in the Author Center of [organicreactions.org](http://organicreactions.org). This file should be used as the style template for drawing text graphics.

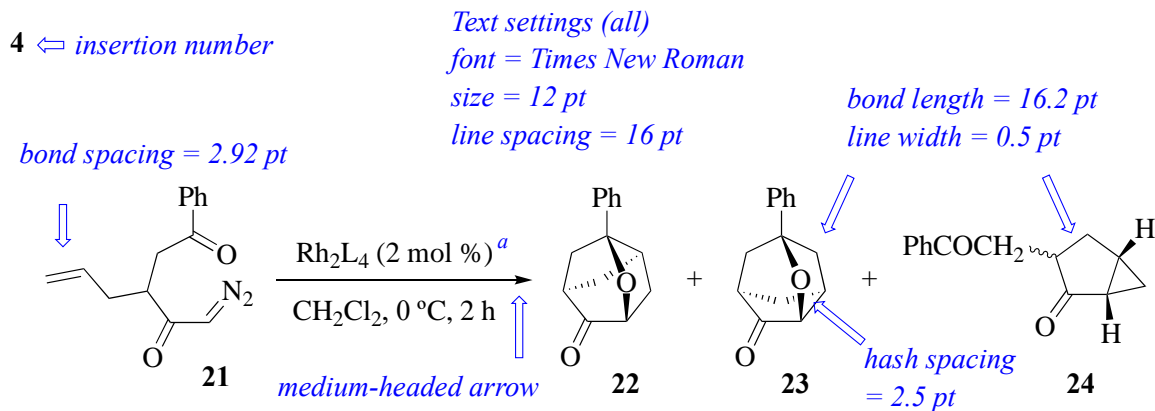
- ✓ To view the document settings, go to the "File" menu and select "Document Settings..."
- ✓ Text graphics should be constructed with the page setup as "US Letter" in "portrait" mode.
- ✓ *The "Drawing" settings are the same in the text graphics and table templates. However, the text font and line spacing settings differ:*

	Times New Roman font size	Captions Line Spacing	Atom Labels Line Spacing
Text graphics	12 pt	fixed 16 pt	fixed 10 pt
Tables	10 pt	fixed 16 pt	fixed 9 pt

## APPENDIX III (continued)

### Annotated Example of a Text Graphic

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



Catalyst	22–24 Yield (%)	22/23/24
Rh <sub>2</sub> (OAc) <sub>4</sub>	94	11:50:39
Rh <sub>2</sub> (cap) <sub>4</sub>	96	13:54:33
Rh <sub>2</sub> (pfb) <sub>4</sub>	87	38:14:48
Rh <sub>2</sub> (tfa) <sub>4</sub>	93	37:13:50

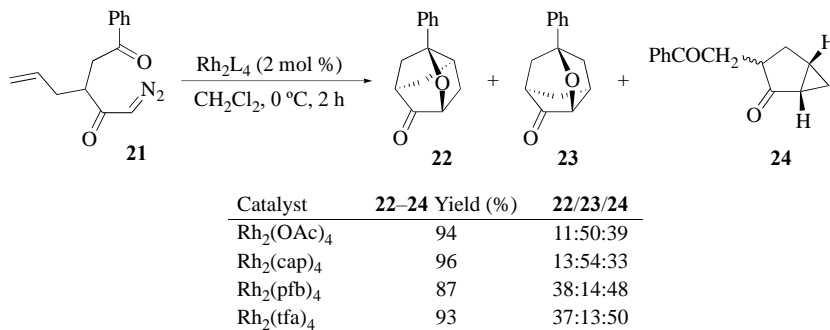
Scheme 5

Preferred maximum 7" (17.8 cm/500 pt)

Absolute maximum 7.25" (18.4 cm/522 pt)

<sup>a</sup> 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:



Scheme 5

## APPENDIX IV: Guidelines for Computer-Drawn Tables and Subtables

Authors are referred to the website [organicreactions.org](http://organicreactions.org) to download instructional videos about preparing table files.

A ChemDraw stationery file (*OR Table Stationery.cds*) is provided via e-mail and is available in the Author Center of [organicreactions.org](http://organicreactions.org). This file should be used as the style template for drawing table entries.

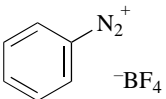
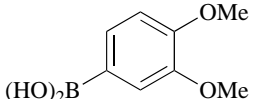
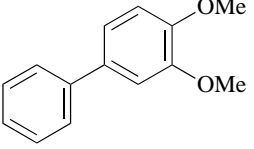
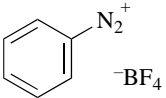
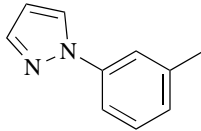
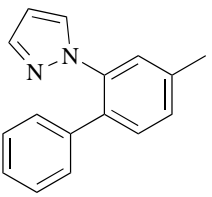
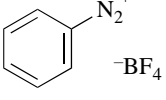
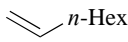
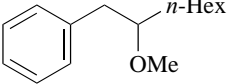
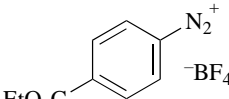
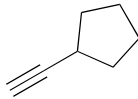
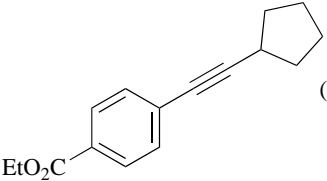
- ✓ To view the document settings, go to the "File" menu and select "Document Settings..."
- ✓ Tables are prepared using US Letter size pages in landscape orientation. Note that "Pages" *NOT* "Poster" is selected in the Layout tab. The multipage feature is *NOT* an option for the preparation of *Organic Reactions* tables.
- ✓ The "Drawing" settings are the same in the text graphics and table templates. However, the font size and line spacing settings differ:

	Times New Roman font size	Captions Line Spacing	Atom Labels Line Spacing
Text graphics	12 pt	fixed 16 pt	fixed 10 pt
Tables	10 pt	fixed 16 pt	fixed 9 pt

### ***Sample Table Files, with Example Deletions and Insertions***

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.

TABLE 6. CROSS-COUPLING OF ARYL DIAZONIUM SALTS

	Redox Partner	Transition Metal Partner	Conditions	Product(s) and Yield(s)	Refs.
	guide marker for eq				
	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.	
<b>Tab06-e001</b> C <sub>6</sub>	 2.0 eq		Ru(bpy) <sub>3</sub> (PF <sub>6</sub> ) <sub>2</sub> (2.5 mol %), Au(PPh <sub>3</sub> )NTf <sub>2</sub> (5 mol %), H <sub>2</sub> O (60 eq), MeCN, CFL (20 W), rt, 16 h	 (83%) {Smith, 2013 #203}	
<b>Tab06-e002</b> C <sub>6</sub>	 4.0 eq		Ru(bpy) <sub>3</sub> Cl <sub>2</sub> •6H <sub>2</sub> O (2.5 mol %), Pd(OAc) <sub>2</sub> (10 mol %), Ag <sub>2</sub> CO <sub>3</sub> (1.0 eq), MeOH, CFL (26 W), 25 °C, 5 h	 (53%) {Jones, 2014 #194}	
<b>Tab06-e003</b> C <sub>6</sub>	 4.0 eq		Fluorescein (5 mol %), MeOH, CFL (23 W), -20 °C, 16 h	 (86%) {Gupta, 2010 #210}	
<b>Tab06-e004</b> C <sub>7</sub>	 4.0 eq		Ru(bpy) <sub>3</sub> (PF <sub>6</sub> ) <sub>2</sub> (0.5 mol %), Au[P(4-MeOC <sub>6</sub> H <sub>4</sub> ) <sub>3</sub> ]Cl (10 mol %), DMF, CFL (23 W), rt, 1 h	 (63%) {Xi, 2009 #201}	

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

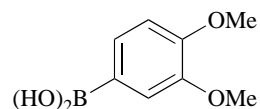
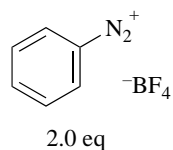
TABLE 6. CROSS-COUPLING OF ARYL DIAZONIUM SALTS

Sample File 2

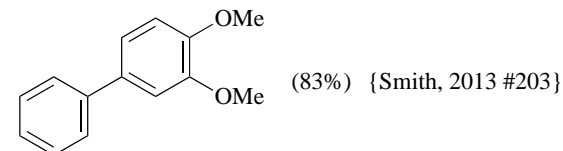
	Redox Partner	Transition Metal Partner	Conditions	Product(s) and Yield(s)	Refs.
--	---------------	--------------------------	------------	-------------------------	-------

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

## Tab06-e001

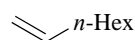
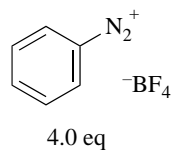
C<sub>6</sub>

Ru(bpy)<sub>3</sub>(PF<sub>6</sub>)<sub>2</sub> (2.5 mol %),  
Au(PPh<sub>3</sub>)NTf<sub>2</sub> (5 mol %), H<sub>2</sub>O (60 eq),  
MeCN, CFL (20 W), rt, 16 h

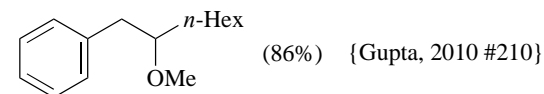


Tab06-e002-deleted ← *Make a note that the entry has been deleted.*

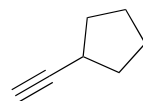
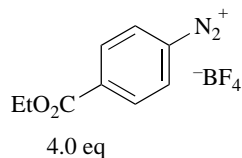
## Tab06-e003

C<sub>6</sub>

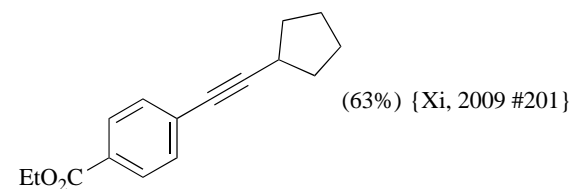
Fluorescein (5 mol %),  
MeOH, CFL (23 W), -20 °C, 16 h



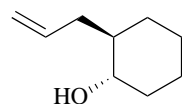
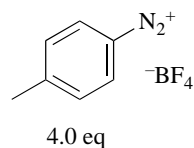
## Tab06-e004

C<sub>7</sub>

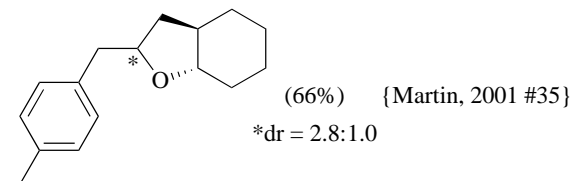
Ru(bpy)<sub>3</sub>(PF<sub>6</sub>)<sub>2</sub> (0.5 mol %),  
Au[P(4-MeOC<sub>6</sub>H<sub>4</sub>)<sub>3</sub>]Cl (10 mol %),  
DMF, CFL (23 W), rt, 1 h



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

C<sub>7</sub>

Ru(bpy)<sub>3</sub>(PF<sub>6</sub>)<sub>2</sub> (2.5 mol %),  
Au(PPh<sub>3</sub>)NTf<sub>2</sub> (10 mol %),  
MeOH, CFL (23 W), rt, 4–16 h





## APPENDIX IV (*continued*)

### *How to Prepare the ChemDraw Table Files*

The following is a transcription of the instructions given in the PowerPoint tutorial found at <https://www.organicreactions.org/video-tutorials/>.

- **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 A, B, etc. and set on a 2<sup>nd</sup> line under the main title. 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 heteroatoms 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<sub>5</sub>, C<sub>6</sub>, 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 subtable, show the count as a range, for example C<sub>5–11</sub>. Put such an entry in the carbon count group of the lowest carbon count (C<sub>5</sub> in this case), and apply the rubric based on the first

subtable entry; i.e., the highest carbon count of the range does not affect where the entry is placed, so C<sub>5-13</sub> can be before C<sub>5-9</sub> and before C<sub>5</sub>.

- **Include carbon counts, starting materials, and products for each entry.**
- **Include only 3 or 4 entries per file**, 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.
- 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 Subtables***

As directed on page 32, subtables 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.

- ✓ Subtables in Table entries should be ordered by the same logic used for ordering of the table entries, e.g., by increasing carbon count.
- ✓ 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 subtable. 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.
- ✓ Each column should be 1 text box. Include the column header (R, Temp (°C), etc.) in the same text box.
- ✓ Use 16-pt line-spacing.

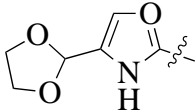
- ✓ Left-align the text in columns that report non-numerical information.
- ✓ Center-align numerical data in columns, such as yield, temperature, and time. For subtables in the tables and text graphics, the “Yield (%)” subheader is used and no parentheses are used around the yield.
- ✓ Select all the columns in the subtable, 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) all components of the subtable. Do not use the bond tool to draw table lines.
- ✓ In both tables and text graphics, if there are different references in a subtable, enter them in the reference column in the same rows as the entries to which they refer.
- ✓ Scale partial structures in subtables 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 subtable, 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., additive, stoich, temp, etc.): — for not reported or not used
- ✓ The connecting atom of a substituent should be consistent within the subtable; i.e., always on the right or always on the left. However, hydrocarbons should always be written in the direct form; e.g., *n*-C<sub>5</sub>H<sub>11</sub>, *c*-C<sub>6</sub>H<sub>11</sub>.

## General Appearance of Properly Constructed Subtables

*In Table Entries* (organized by carbon count)

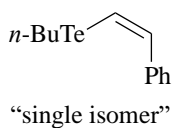
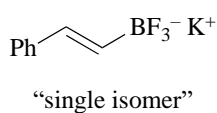
R	Temp (°C)	Time (h)	Yield (%)		
			I + II	I/II	
Me	35	3	96	2.7:1	{Hong, 2004 #952}
Me	80	1	89	4.2:1	{Takahashi, 2003 #960}
Ph	101	24	68	—	{Korotchenko, 2004 #942}

*In Text Graphics*

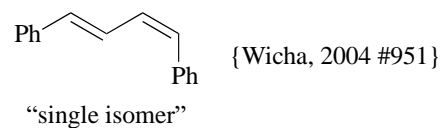
R	Temp (°C)	Time (h)	Yield (%)		Refs
			6 + 7	6/7	
MeO <sub>2</sub> C	25	4.7	60	5.8:1	{Raju, 2006 #63}
BnO(CH <sub>2</sub> ) <sub>2</sub>	25	3	75	9.1:1	{Raju, 2006 #63}
allyl	25	3	70	3.0:1	{Raju, 2006 #63}
	80	3	65	15:1	{Nakadaira, 1972 #195}
( <i>E</i> )-PhCH=CH	80	4.5	66	10:1	{Nakadaira, 1972 #195}

### Example 1: Subtable of Different Conditions

C<sub>8</sub>



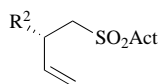
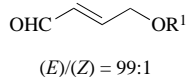
Pd(PPh<sub>3</sub>)<sub>4</sub> (20 mol %),  
base (2 eq), additive (2 eq),  
MeOH, ultrasound, 23 °C, 20 min



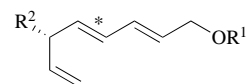
Base	Additive	Yield (%)
K <sub>2</sub> CO <sub>3</sub>	Ag <sub>2</sub> O	65
Cs <sub>2</sub> CO <sub>3</sub>	Ag <sub>2</sub> O	67
Et <sub>3</sub> N	Ag <sub>2</sub> O	66
Et <sub>3</sub> N	AgOAc	84

## Example 2: Subtable of Simple Analogs

C<sub>4</sub>



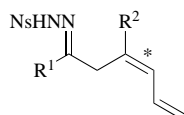
1. MN(SiMe<sub>3</sub>)<sub>2</sub> (1.2 eq), solvent, -78 °C, 30 min
2. Aldehyde (*x* eq); then to rt, 1 h



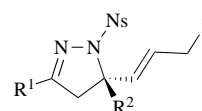
R <sup>1</sup>	R <sup>2</sup>	Act	M	Solvent	<i>x</i>	Yield (%)	*( <i>E</i> )/( <i>Z</i> )	
PMB	Me	PT	Li	DME	1.0	71	84:16	{ Gaertner, 2013 #1891 }
TBDPS	Me	BT	Li	DME	1.1	88	88:12	{ Gaertner, 2013 #1891 }
PMB	Et	PT	K	THF	1.5	58	69:31	{ Ulver, 2006 #503 }

example from a different Table:

C<sub>13–22</sub>



- C10** (0.1 eq), NIS (1.2 eq),  
toluene/CH<sub>2</sub>Cl<sub>2</sub> (3:1), 4 Å MS,  
-80 °C, 72 h



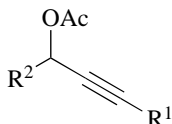
{ Tripathi, 2015 #43 }

*Config	R <sup>1</sup>	R <sup>2</sup>	Yield (%)	er
( <i>Z</i> )	<i>c</i> -C <sub>6</sub> H <sub>11</sub>	Me	43	67.0:33.0
( <i>E</i> )	<i>c</i> -C <sub>6</sub> H <sub>11</sub>	Ph	66	95.0:5.0
( <i>E</i> )	Ph	Me	61	96.5:3.5

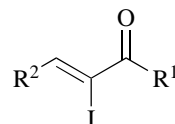
## Example 3: Subtable Ordering of Structures with Variable R<sup>1</sup> and R<sup>2</sup>

*Note that ordering within the subtable is first by R<sup>1</sup>, then by R<sup>2</sup>.*

C<sub>13–16</sub>



- NIS (2.2 eq), MeCN/H<sub>2</sub>O (1:1), 100 °C

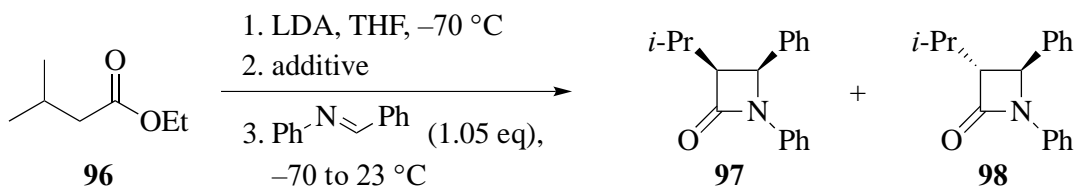


(*Z*)/(*E*) > 99:1

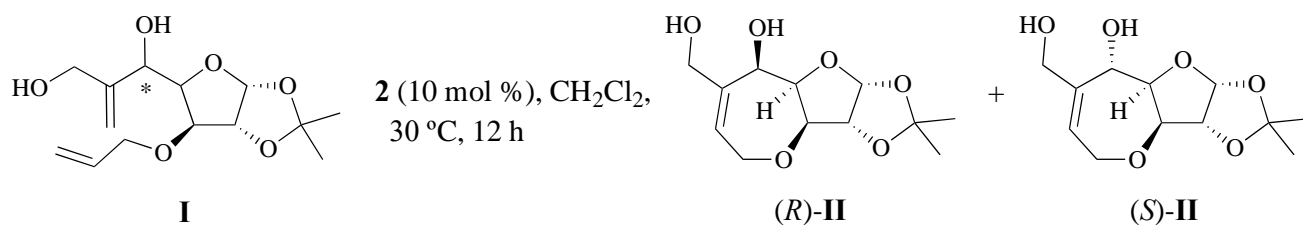
R <sup>1</sup>	R <sup>2</sup>	Time (h)	Yield (%)
Ph	2-furyl	3	77
Ph	<i>c</i> -C <sub>6</sub> H <sub>11</sub>	5	83
Ph	2,3-Cl <sub>2</sub> C <sub>6</sub> H <sub>3</sub>	4	75
Ph	2-MeC <sub>6</sub> H <sub>4</sub>	18	65
4-FC <sub>6</sub> H <sub>4</sub>	Ph	4.5	79
4-MeC <sub>6</sub> H <sub>4</sub>	Ph	4	85

### Example 4: Subtable of Isomers

*Note that if the major product changes in a subtable, each of the major isomers must be drawn.*



Additive	Yield (%)	
	97 + 98	97/98
—	88	99:1
HMPA	92	6:94



*Isomer I	(R)-II	(S)-II
(R)	(84)	(0)
(S)	(0)	(92)

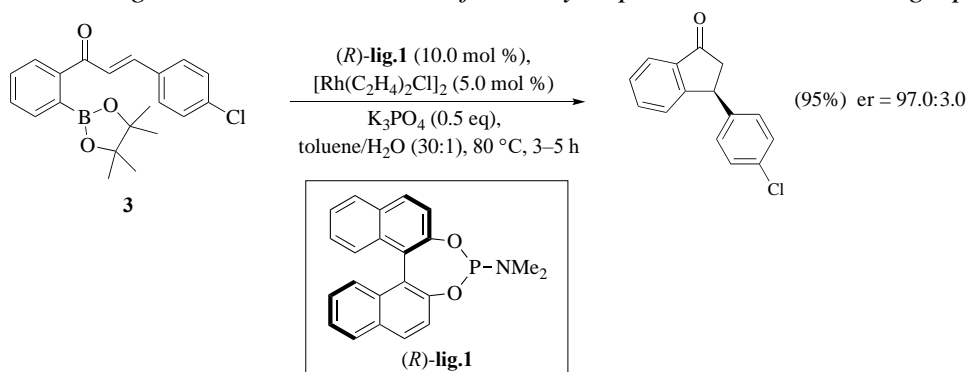
## APPENDIX V: Ligand/Catalyst Numbering

- 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*-**L**” (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.*

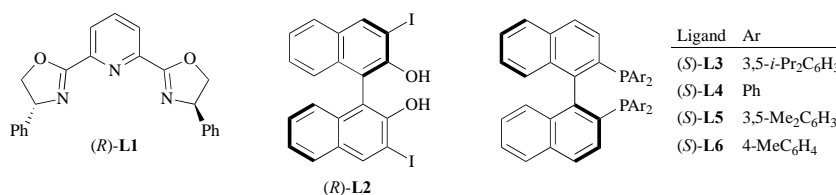


Scheme 10

### 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. If subtables are used to group similar structures in the Chart, the numbering must be contiguous within the subtable.
- ✓ Use the notation **Lx** and **Cx**.
- ✓ The ligand/catalyst structure should not be drawn in the first table entry in which it is used.

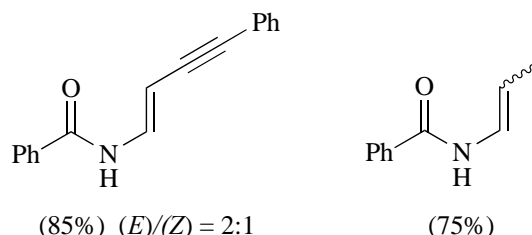
CHART 1. LIGANDS USED IN THE TABLES



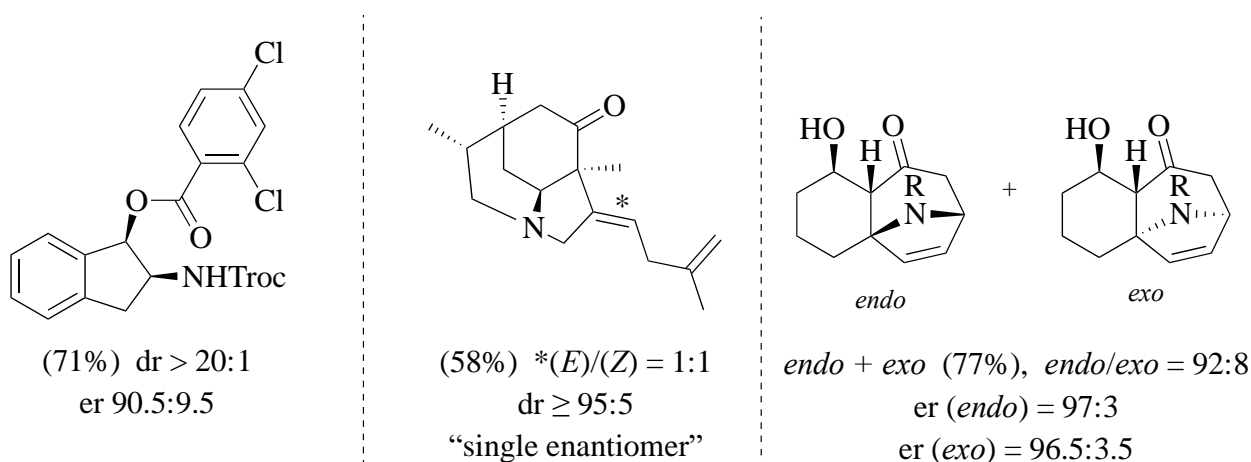
## APPENDIX VI: Guidelines for Stereochemical Depictions

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.

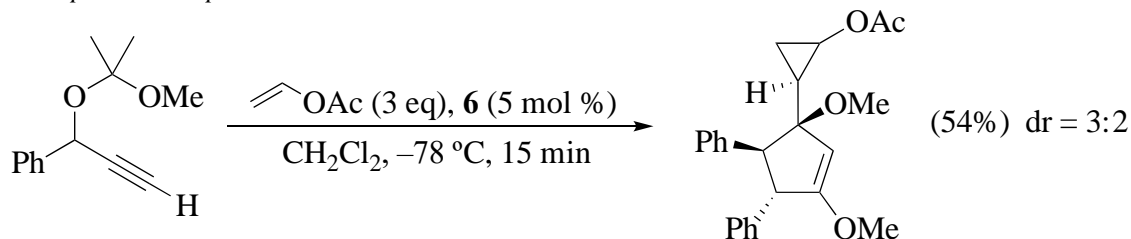


- Draw the major isomer when the product is a mixture of isomers with specified composition and known configuration. Structures of minor isomers may be included if necessary for clarity.



- 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.

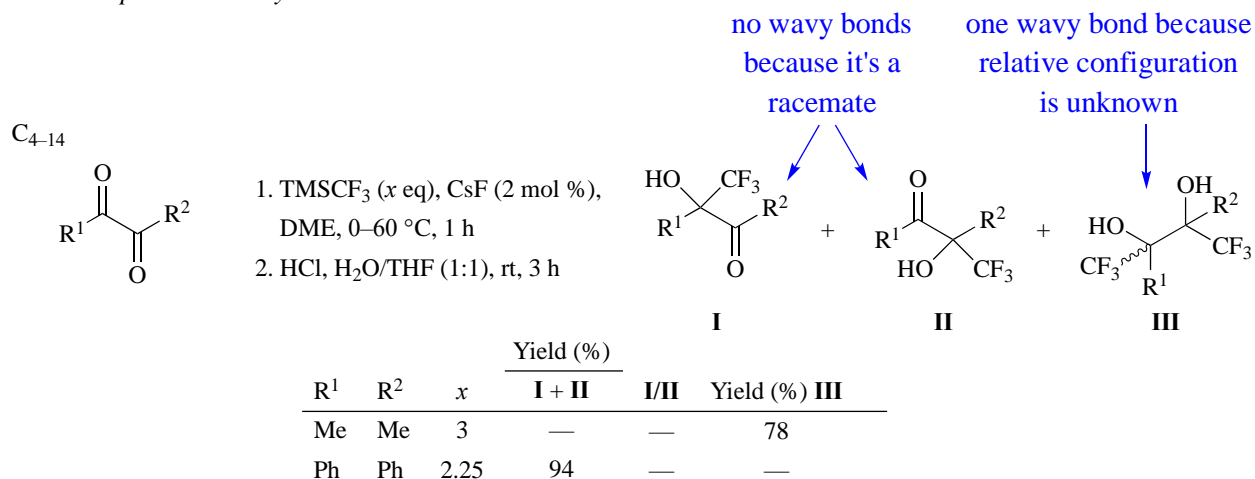
Example Text Graphic





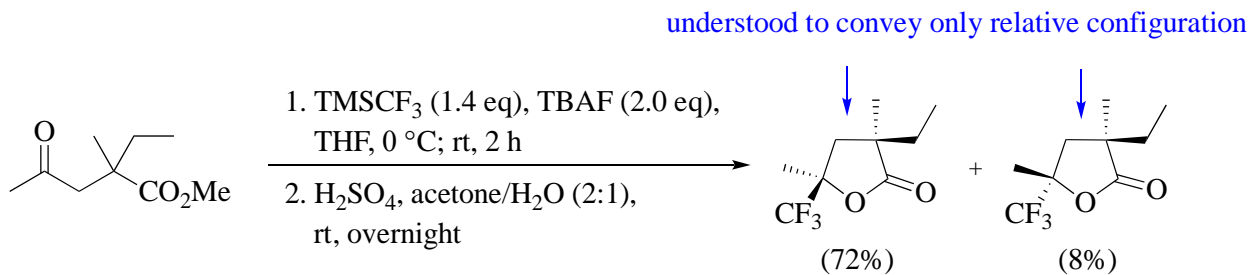
- Use a wavy line for the key bond when the product is a mixture of unknown composition.

*Example Table Entry*



- 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 starting materials 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:

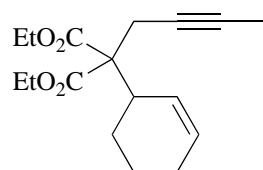
major diastereomer

configuration unspecified

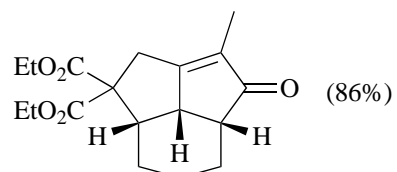
“single enantiomer”, “single diastereomer” (with quotation marks)

- See “Reporting Regioisomeric and Stereochemical Ratios” section for specific rules for using these terms.

C<sub>13</sub>

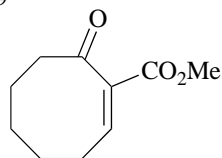


**C6** (10 mol %),  
CO (0.34 atm),  
toluene, 90 °C

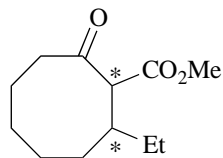


“single diastereomer”

C<sub>9</sub>



(*S,S*)-**OP186** (10 mol %),  
Cu(OTf)<sub>2</sub> (10 mol %),  
ZnEt<sub>2</sub> (3 mol %),  
CH<sub>2</sub>Cl<sub>2</sub>, 23 °C, 17 h



(65%) er = 99.0:1.0

\* rel and abs config undetermined

## APPENDIX VII: Styles for Selected Abbreviations and Symbols

<u>USE</u>	<u>INSTEAD OF</u>
Me, Et	CH <sub>3</sub> ,CH <sub>3</sub> CH <sub>2</sub>
<i>i</i> -Pr, <i>t</i> -Bu	(CH <sub>3</sub> ) <sub>2</sub> CH, (CH <sub>3</sub> ) <sub>3</sub> C, <i>i</i> Pr, <i>t</i> Bu
<i>n</i> -C <sub>6</sub> H <sub>13</sub>	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub>
4-MeC <sub>6</sub> H <sub>4</sub> , 3-Cl-4-MeC <sub>6</sub> H <sub>3</sub>	<i>p</i> -MePh, <i>m</i> -Cl- <i>p</i> -MeC <sub>6</sub> H <sub>3</sub>

### Abbreviations for cyclic substituents:

cyclopentyl	<i>c</i> -C <sub>5</sub> H <sub>9</sub>
cyclohexyl	<i>c</i> -C <sub>6</sub> H <sub>11</sub> or Cy
naphthyl	1-Np or 2-Np
pyridyl	Py
tolyl	Tol

### Use the following forms:

4 Å MS  
 2 N HCl  
 0.5 M HCl (in MeOH)  
 Na<sub>2</sub>SO<sub>4</sub>•10H<sub>2</sub>O  
 aq NaOH  
 mol %  
*hν*

## SHORTCUTS FOR COMMONLY USED SYMBOLS AND SIGNS

Symbol	Mac Shortcut	PC Shortcut*	Example
°	shift-option-8 or option-0	Alt-0176	23 °C
•	option-8	Alt-0149	BF <sub>3</sub> •OEt <sub>2</sub>
-	hyphen		<i>N</i> -acetyl, <i>t</i> -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		<i>hν</i>
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

\*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](http://pubs.acs.org/userimages/ContentEditor/1218717864819/joceah_abbreviations.pdf)

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

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

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

$$\text{er} = [(100 + \% \text{ee})/2]: [(100 - \% \text{ee})/2]$$