

Scientific Writing

I. Manuscript Structure

Dr. Wujian Miao



Outline

- I. Manuscript Structure
- II. Vigorous Writing
- III. Writing Style and Punctuation
- IV. Word Usage, Sentences, and Paragraphs
- V. Schemes, Figures, and Tables (ChemDraw and OriginLab)
- VI. Conventions in Chemistry
- VII. Reference Citations-EndNote



Key References of the Course

1. Coghill, A. M., Garson, L. R. & American Chemical Society. *The ACS Style Guide: Effective Communication of Scientific Information* (American Chemical Society; Oxford University Press, Oxford ; New York, 2006).
2. Ebel, H. F., Bliedert, C. & Russey, W. E. *The Art of Scientific Writing: From Student Reports to Professional Publications in Chemistry and Related Fields* (VCH, Weinheim, Federal Republic of Germany; New York, NY, USA, 1987).
3. Mecaskill, M. K. *Grammar, Punctuation, and Capitalization: A Handbook for Technical Writers and Editors* (NASA; United States, Washington, United States, 1990).
4. Robinson, M. S., Stoller, F. L., Costanza-Robinson, M. & Jones, J. K. *Write Like a Chemist: A Guide and Resource* (Oxford University Press, USA, Oxford, 2008).
5. Strunk, W. & White, E. B. *The Elements of Style* (Pearson Longman, New York, 2009).



Manuscript Structure for chemistry related journals

- Title (with Author(s) and author bylines)
 - Abstract
 - Main Text
- I. Introduction
 - II. Experimental Section
 - III. Results and Discussion
 - IV. Conclusions
 - V. Acknowledgements
 - VI. References
 - VII. Schemes, Figures, and Tables
- Supporting Information



- Title – Short, descriptive phrase. Use specific and informative titles with a high keyword content.
 - Author(s) and author bylines
- I. Give authors' full names, the complete mailing address of the place where the work was done, and the current addresses of the authors, if different, as a footnote.
 - II. Indicate the corresponding author by an asterisk and provide an e-mail address, phone, and fax number for that person.

analytical chemistry an article in pubs.acs.org

Sensitive Determination of Triacetone Triperoxide Explosives Using Electrogenerated Chemiluminescence

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Title Examples

- Original:** Action of antibiotics on bacteria
Revised: Inhibition of growth of *Mycobacterium tuberculosis* by streptomycin
Comments: Titles should be specific. Think about “how will I search for this piece of information” when you design the title.
- Original:** Fabrication of carbon/CdS coaxial nanofibers displaying optical and electrical properties via electrospinning carbon
Revised: Electrospinning of carbon/CdS coaxial nanofibers with optical and electrical properties
Comments: The title is nonsense. All materials have properties of all varieties. You could examine my hair for its electrical and optical properties! You MUST be specific.
- Long title distracts readers. Remove all redundancies such as “studies on,” “the nature of,” etc. Never use expressions such as “preliminary.” Be precise.



• **Abstract**

- a. Very concise summary of main result(s) (< 250 words)
- b. Most widely read portion of the paper
- c. Most journal indexes only list the abstract

• **Introduction**

- a. Identify issue or problem to be addressed
- b. Provide context (historical and/or within particular field)
- c. Summarize approach
- d. Compare/contrast with previous work
- e. Answer the question: Why is this important or interesting?
- f. Lots of references



Experimental Section

a. **Chemicals and Materials (Safety considerations)**

b. **Instrumentation/apparatus/system**

- i. Often a diagram is necessary
- ii. Give enough detail for readers to get a mental picture
- iii. Reference previous work (perhaps your own) that used same or similar apparatus

c. **Procedure**

- i. Give enough detail for an expert reader to repeat the experiment
- ii. Try to make this section as accessible as possible to the non-expert
- iii. Emphasize only the crucial points
- iv. Published procedures should be cited



Results and Discussion

• **Results**

- i. Should complement graphical information (figures and tables)
- ii. Comment on qualitative and quantitative information in graphs
- iii. If needed, discuss unusual aspects of figures (e.g. nonlinear scales)

• **Discussion**

- i. Relevance of results
- ii. Analysis procedure
- iii. Comparison with other work
- iv. Unusual aspects of data
- v. Be concise and deal with the interpretation



Conclusions

- a. Re-state importance of results or experiment
- b. Do not repeat information already presented in the text or abstract.
- c. Make sure the statement is supported by the data presented in the text.
- d. Hint at future directions or improvements or point out those that are underway.
- e. Correlate to the objectives included in the introduction.



Acknowledgements

- May acknowledge technical assistance, gifts, the source of special materials, financial support, meeting presentation information.
- If the article is dedicated to another scholar, a brief statement, such as “This article is dedicated to [name]”, can be included.
- Statements about author contributions to the work or equal contributions of work should be included as a separate statement.



References

- a. Numbered as they appear in text
- b. Should all follow the same style (depending on the requirements of a specific journal)
- c. Use of Endnote is strongly recommended
- d. Manually editing often needed
- e. Avoid excessive self-citations and excessive citations of publications from the same region

Example of an ACS paper citation:

- (1) Ho, M.; Pemberton, J. E. *Anal. Chem.* **1998**, *70*, 4915–4920.
- (2) Bard, A. J.; Faulker, L. R. *Electrochemical Methods*, 2nd ed.; Wiley: New York, 2001.



Schemes, Figures, and Tables

- a. The most important part of a paper!
- b. The point of the paper should be obvious from Schemes, figures, and tables alone.
- c. Captions are descriptive, self-explanatory, but not lengthy.
- d. Work hard to make them nice to look at, informative, and compact.
- e. Consistently sizing letters and labels in graphics throughout your manuscript.
- f. Do not use figures or tables that duplicate each other or material already in the text.



Supporting Information (SI)

- Additional examples of experimental and theoretical figures
- Extensive figures connected with computational modeling, analytical and spectral characterization data for new compounds
- Extensive instrument and circuit diagrams
- Detailed mathematical derivations, computation procedures, and programs
- SI is subject to peer review.
- SI is also indexed and abstracted by the CA



Order of Manuscript Preparation

1. Prepare the **schemes, figures, and tables**.
2. Write the **Experimental Section**.
3. Write up the **Results and Discussion**. Finalize the Results and Discussion before writing the introduction. This is because, if the discussion is insufficient, how can you objectively demonstrate the scientific significance of your work in the introduction?
4. Write a clear **Conclusion**.
5. Write a compelling **Introduction**.
6. Write the **Abstract**
7. Compose a concise and descriptive **Title**.
8. Select 3-5 **Keywords** for indexing.
9. Write the **Acknowledgements**.
10. Edit and finalize the **References**.



Publication and Peer Review

Publication Procedure (6-12 months)

1. Author submits →
2. Editor is assigned to manuscript →
3. Editor assigns reviewers to inspect →
4. Reviewers decide on whether to review paper →
5. Several reviewers inspect and edit →
6. Editor decides on accuracy of reviews and whether to accept paper →
7. If accepted, editor sends paper back to author with revisions →
8. Author revises paper and sends it back →
9. Possibility of second review process →
10. Proof reading →
11. Publish on line →
12. Publish in printing format.



Scientific Misconduct

- Gift Authorship
- Redundant Publication (repeated publication)
- Plagiarism (“turnitin” database)
<http://turnitin.com/>
- Fabrication
- Falsification
- Conflict of Interest
- List of fake reviewers



Tips and Tricks

- Find out and read carefully the updated *Author’s Guideline* from journal’s website
- Learn from the published papers of the journal
- If needed, use “Template for Submission of Manuscripts to xxx Journals”



Journal article move structures

Abstract


1. State What Was Done

1.1 Identify the research area and its importance (optional)
 1.2 Mention a gap addressed by the work (optional)
 1.3 State purpose and/or accomplishment(s) of work

2. Identify Methods Used
(i.e., procedures and/or instrumentation)

3. Report Principle Findings

3.1 Highlight major results (quantitatively or qualitatively)
 3.2 Offer a concluding remark (optional)



Introduction

1. Introduce the Research Area

1.1 Identify the research area
 1.2 Establish the importance of the research area
 1.3 Provide essential background information about the research area

2. Identify a Gap (or Gaps)


3. Fill the Gap

3.1 Introduce the current work
 3.2 Preview key findings of the current work (optional)

General

↓

Specific



Cite relevant literature

Methods

1. Describe Materials
(e.g., materials, chemicals, samples, cultures, sampling sites, general reaction conditions)


2. Describe Experimental Methods

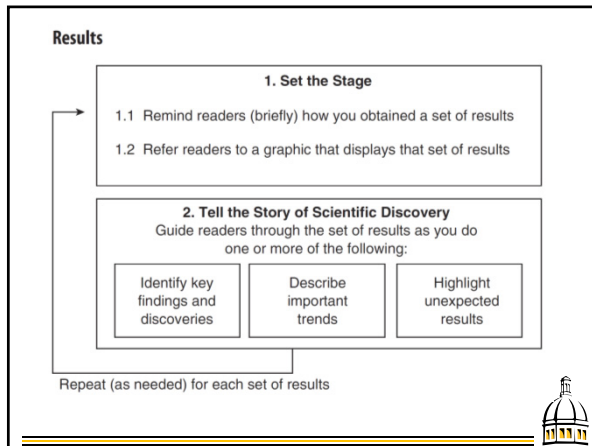
Describe procedure(s)

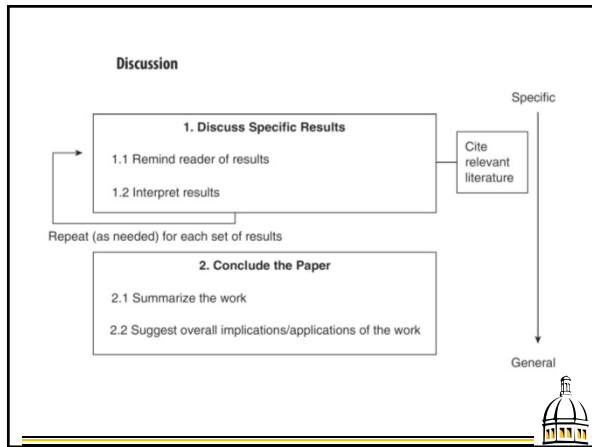
↔

Describe instrumentation

3. Describe Numerical Methods (if applicable)
(e.g., statistical analyses, theoretical computations)







Scientific Writing

II. Vigorous Writing

Dr. Wujian Miao



What makes good writing?

Why do we care about scientific writing?

“A research project is not completed until the result is published” -- Alan J Bard

- Good writing communicates an idea clearly and effectively.
- Good writing is elegant and stylish.

For a scientist like us:

- Having something to say.
- Logical and clear thinking.
- A few simple, learnable rules of style (the tools we'll learn in this class).



Clear writing starts with clear thinking

- Before you start writing, ask:
“What am I trying to say?”
- When you finish writing, ask:
“Have I said it?”
- Once you know what you're trying to say, then pay attention to your words!



Vigorous writing

- Vigorous writing is concise.
 - A sentence should contain no unnecessary words.
 - A paragraph no unnecessary sentences.
 - A drawing should have no unnecessary lines.
-
- Requires the writer
 - a. Make all the sentence short
 - b. Avoid all detail and treat the subjects only in outline
- Thus, **Every Word Tells**.



To write well

Words:

1. Reduce dead weight words and phrases
2. Cut, cut, cut; learn to part with your words
3. Be specific

Sentences:

4. Follow: subject + verb + object (*SVO*)
5. Use strong verbs and avoid turning verbs into nouns
6. Eliminate negatives; use positive constructions instead



Examples

• 1. Original:

I would like to assert that the author should be considered to be a buffoon.

Better:

The author is a buffoon.

• 2. Original:

The expected prevalence of mental retardation, based on the assumption of a normal distribution of intelligence in the population, is stated to be theoretically about 2.5%.

Better:

The expected prevalence of mental retardation, if intelligence is normally distributed, is 2.5%.



Original:

This paper provides a review of the basic tenets of cancer biology study design, using as examples studies that illustrate the methodologic challenges or that demonstrate successful solutions to the difficulties inherent in biological research.

Better:

This paper reviews cancer biology study design, using examples that illustrate specific challenges and solutions.



Original:

As it is well known, increased athletic activity has been related to a profile of lower cardiovascular risk, lower blood pressure levels, and improved muscular and cardio-respiratory performance.

Revisions:

Increased athletic activity is associated with lower cardiovascular risk, lower blood pressure, and improved fitness.

Or just:

Increased athletic activity is associated with improved cardiovascular health.

Or, use verbs:

Increased athletic activity reduces cardiovascular risk and improves cardiovascular performance.



Hunt down and cast out all unneeded words that might slow your readers

Very, really, quite, basically, generally

These words seldom add anything useful. Try the sentence without them and see if it improves.

Watch out for the verb “to be”

Often “there are” is extra weight.

There are many students who like writing.

- Many students like writing.



Dead weight phrases to avoid

- in the event that
- in the nature of
- it has been estimated that
- it seems that
- the point I am trying to make
- what I mean to say is
- it may be argued that
- for the most part
- for the purpose of
- in a manner of speaking
- in a very real sense
- in my opinion
- in the case of
- in the final analysis



► Omit empty phrases such as

- As already stated
- It has been found that
- It has long been known that
- It is interesting to note that
- It is worth mentioning at this point
- It may be said that
- It was demonstrated that



Omit excess words


Instead of	Use
It is a procedure that is often used.	This procedure is often used.
There are several steps that must be completed.	Several steps must be completed.
This is a problem that is...	This problem is...
These results are preliminary in nature.	These results are preliminary.



Example

poor writing:
 "The main theme of this section is to tell why we have chosen to generalise..."


economical writing:
 "This section presents our rationale for generalising..."



Example


poor writing:
 "Our purpose has been to provide a description of thermodynamic phase transition ..."

economical writing:
 "We have tried to describe thermodynamic phase transition..."




Use single words instead of phrases


Instead of	Use
a number of	many, several
a small number of	a few
are in agreement	agree
are found to be	are
are known to be	are
at present	now
at present time	now
based on the fact that	because




Instead of	Use
by means of	by
despite the fact that	although
due to the fact that	because
fewer in number	fewer
for the reason that	because
has been shown to be	is
if it is assumed that	if
in color, e.g., red in color	<i>Just state the color, e.g., red</i>
in length	long




Instead of	Use
in consequence of this fact	therefore, consequently
in order to	to
3-mm in diameter	3-mm diameter
In shape, e.g., round in shape	<i>just state the shape, e.g., round</i>
in size, small in size	<i>just state the size, e.g., small</i>
in spite of the fact that	although
in the case of	in..., for...



Instead of	Use
in view of the fact that	because
is known to be	is
it appears that	apparently
it is clear that	clearly
it is possible that	possibly
of great importance	important
on the order of	about
owing to the fact that	because
prior to	before
reported in the literature	reported




Instead of	Use
subsequent to	after
a majority of	most
are the same opinion	agree
at the present moment	now
less frequently occurring	rare
all three of the	the three
give rise to	cause
in a position to	can
in all cases	always
in close proximity	near




Example

poor (wordy)	better (economical)
place under consideration	consider
perform an experiment	experiment
present a discussion of	discuss
conduct an investigation	investigate
make an attempt	try
introduce a replacement	replace
for the case of	for
in many cases	often
it has rarely been the case that we	we rarely
in the case when	when




Beware of clunky words that sneak in


Beware of	Use instead
assistance	help
utilize	use
numerous	many
facilitate	ease
individual	Man or woman
remainder	rest
initial	first
implement	do
sufficient	enough




Beware of	Use instead
attempt	try
referred to as	called
with the possible exception of	except
He totally lacked the ability to	He could not
until such time as	until
investigate	study
initiate	start
indicate	show



Beware of	Use instead
currently	now
facilitate	help
endeavor	try
ascertain	Find out
3 am in the morning	3 am
absolutely spectacular	spectacular
a scientist who is honest	An honest scientist
A total of 14 chemicals	14 chemicals
circle around	circle




Wordy vs To the point	
Wordy	To the point
completely unanimous	unanimous
consensus of opinion	consensus
each and every study	each study
end result	result
he is a man who	he
new innovations	innovations
a period of four days	four days
repeat again	repeat
shorter/longer in length	shorter/longer



Wordy	To the point
surrounded on all sides	surrounded
there is no doubt but that	undoubtedly
unexpected surprise	surprise


- Ask yourself, is this word or phrase necessary?
- What happens if I take it out?
- Most of the time, you'll find you don't need it!



Do not be afraid to cut

Original:
It has been reported that brain injury incidence shows two peak periods in almost all reports: rates are the highest in young people and the elderly.


Revision:
Brain injury incidence peaks in the young and the elderly.



Do not use contractions in scientific papers

INCORRECT
The identification wasn't confirmed by mass spectrometry.

CORRECT
The identification was not confirmed by mass spectrometry.



Do not use the word “plus” or the plus sign as a synonym for “and”

Incorrect:

Two bacterial enzymes were used in a linked-enzyme assay for heroin plus metabolites.

Correct:

Two bacterial enzymes were used in a linked-enzyme assay for heroin and its metabolites.



Do not use “respectively” when you mean “separately” or “independently”

Incorrect:

The electrochemical oxidations of chromium and tungsten tricarbonyl complexes, respectively, were studied.

Correct:

The electrochemical oxidations of chromium and tungsten tricarbonyl complexes were studied separately.



Do not use a slash to mean “and” or “or”

Incorrect:

Hot/cold extremes will damage the samples.

Correct:

Hot and cold extremes will damage the samples.



Replace “and/or” with either “and” or “or”, depending on your meaning

Incorrect: Our goal was to confirm the presence of the alkaloid in the leaves and/or roots.

Correct: Our goal was to confirm the presence of the alkaloid in the leaves and roots.

Also correct: Our goal was to confirm the presence of the alkaloid in either the leaves or the roots.

Also correct: Our goal was to confirm the presence of the alkaloid in the leaves, the roots, or both.



Avoid using the word “recently”

Your article or book may be available for a long time. This word will make it look dated in little time.

Poor:

It was recently found that these effects enhance the bond strength.

Better:

Harris and Harris (2006) found that these effects enhance the bond strength.



Gender-neutral language

Instead of “man”, use “people”, “humans”, “human beings”, or “human species”, depending on your meaning.

Outdated: The effects of compounds I-X were studied in rats and man.

Gender-neutral: The effects of compounds I-X were studied in rats and humans.



Outdated: Men working in hazardous environments are often unaware of their rights and responsibilities.

Gender-neutral: People working in hazardous environments are often unaware of their rights and responsibilities.

Outdated: Man's search for beauty and truth has resulted in some of his greatest accomplishments.

Gender-neutral: The search for beauty and truth has resulted in some of our greatest accomplishments.



Instead of “manpower”, use “workers”, “staff”, “work force”, “labor”, “crew”, “employees”, or “personnel”, depending on your meaning.

Instead of “man-made”, use “synthetic”, “artificial”, “built”, “constructed”, “manufactured”, or even “factory-made”.



Instead of “wife”, use “family” or “spouse” where appropriate.

Outdated: The work of professionals such as chemists and doctors is often so time-consuming that their wives are neglected.

Gender-neutral: The work of professionals such as chemists and doctors is often so time-consuming that their families are neglected.

Outdated: the society member and his wife

Gender-neutral: the society member and spouse



Scientific Writing

III. Writing Style and Punctuation

Dr. Wujian Miao



Writing style

Every writer has a personal style, but all good writing tends to observe guidelines and conventions that communicate meaning clearly and exactly to readers. Scientific writing, in particular, must be precise and unambiguous to be effective.



Questions for Drafting Your Manuscript

- a. What is the function or purpose of this manuscript?
Are you describing original and significant research results? Are you reviewing the literature? Are you providing an overview of the topic?
- b. Who is the audience? Why would they want to read your manuscript? What will you need to tell them to help them understand your work?
- c. How is your work different from that described in other reports on the same subject?
- d. What is the best format for publishing this manuscript—as a journal article, book, or book chapter? If you choose a journal article, which journal is most appropriate?



Verbs: Voice

► Use the active voice when it is less wordy and more direct than the passive.

Poor: The fact that such processes are under strict stereoelectronic control is demonstrated by our work in this area.

Better: Our work in this area demonstrates that such processes are under strict stereoelectronic control.



► Use the passive voice when the doer of the action is unknown or not important or when you would prefer not to specify the doer of the action.

The solution *is shaken* until the precipitate forms.

Melting points and boiling points *have been approximated*.

Identity specifications and tests *are not included* in the monographs for reagent chemicals.



Verbs: Tense

In general, these are the verb tenses typically used in the following sections of a research paper:

Title: does not need to be a complete sentence, and no verb is necessary. Otherwise, uses the simple present tense.

Abstract: past tense

Introduction: mixed

- when stating a fact that is widely accepted, the present tense is appropriate.



e.g., DNA is composed of four nucleotides.

- When referring to a previous study with results that are still relevant, use the present perfect tense (“have shown”, has been shown”)

e.g., Johnson et al. have shown that quantum dots can be used as ECL labels for quantification of biomolecules.

- Note that the present tense is used when a specific result, figure, or paper is the subject of a sentence.

e.g., The results of their study indicate that the method is highly sensitive.



- When referring specifically to the methods used in a previous paper, the past tense is best.

e.g., Smith et al sampled 6 lake water samples and determined their mercury concentrations.

- Statements that are no longer considered true should remain in the past tense.

e.g., Early physicists thought that electrons traveled in defined orbits



- At times, a combination of tenses is necessary:

e.g., Robert Corey suggested [past] that DNA contained three helices, but subsequent work has proved [present perfect] the existence of a double-helix structure.

Theory: present tense

Experimental (Methods): past tense, as reporting what was done during the study

e.g., All electrochemical experiments were performed with a computerized electrochemical workstation (CH Instruments, Austin, TX, USA).



- When one action occurred before another, the past perfect tense (“had verb-ed”) can be used to indicate the earlier action, with the subsequent action in the simple past tense.

e.g., Acetonitrile was dried by passing a column containing alumina powders that had been heated at 200 °C for 3 hrs and then cooled down to room temperature.

- In rare cases in which one action occurred while another was ongoing, the past progressive (“was or were + verb-ing”) is used.

e.g., While the solutions were incubating [past progressive], the temperature was raised [past] 1°C per hour.



Results: largely past tense

Because the experiments described in the text were completed before the paper was written.

e.g., we detected no fluorescence in the control sample.

- In certain cases, however, the present tense is needed. For example, when referring to the entire paper or to individual elements of the manuscript (e.g., figures, tables, sections, results, or data).

e.g., 1. Our results demonstrate that magnesium is essential for enzymatic function.

2. Figure 1 shows our fluorescence data.

3. In this study, we report the effect of carbon nanotubes on the ECL quenching of the Ru(bpy)₃²⁺/TPPrA system.



Discussion: often alternates between past tense (when discussing results of current study: “we found”) and present tense (“our results are consistent with” or “the theory of natural selection predicts that”).

Conclusions: mixed. (past + present + future)

e.g., 1. Effects of CNTs on the ECL behavior of CdTe QDs using TPPrA and DBAE as the anodic coreactant were investigated.

2. We conclude that Ag/AgCl reference electrode is not suitable for study of catalytic oxidation of formic acid fuel cells.

3. The methods reported here will allow for rapid screening in the field.



► Present and simple past tenses may both be correct for results, discussion, and conclusions.

- The characteristics of the voltammetric wave **indicate** that electron transfer occurs spontaneously.
- The absence of substitution **was confirmed** by preparative-scale electrolysis.

The **use** of present or simple past tense for results, discussion, and conclusions **should be consistent** within a paper.



Punctuation

- Comma ,
- Colon :
- Period .
- Quotation marks “ ”, ‘ ’
- Hyphen -, en dash –, and em dash —
- Semicolon ;
- Parentheses ()
- Square brackets []
- Ellipsis point ...



Comma

• In a series of three or more terms with a single conjunction, use a comma after each term except the last.

e.g.,

- red, white, and blue
- Water, sodium hydroxide, and ammonia were the solvents.
- The red needles were collected, washed with toluene, and dried in a vacuum desiccator.



- a. Several experimental parameters need to be finalized, which include initial potential, final potential, **and** scan rate.
- b. The compound does not add bromine, undergo polymerization by the Diels–Alder reaction, **or** react with electrophiles
- c. Pressures at the bulkhead, in the cove, **and** at the seal were measured.



EXPERIMENTAL SECTION

Chemicals

4-Aminobenzoic acid (4-ABA, 99%), 4-morpholineethanesulfonic acid (MES, $\geq 99\%$), 1-methylimidazole (99%), ethylenediamine (En, $\geq 99.5\%$) lithium perchlorate (LiClO_4 , $\geq 95\%$), **and** potassium ferricyanide(III) ($\text{K}_3\text{Fe}(\text{CN})_6$, $\geq 99\%$) were purchased from Sigma-Aldrich (Saint Louis, MO, USA). Sodium phosphate monobasic monohydrate ($\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$, $\geq 99\%$), potassium chloride (KCl , $\geq 99\%$), **and** sodium bicarbonate (NaHCO_3) were received from J.T. Baker Chemicals Co. (Phillipsburg, NJ, USA). 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC), N-hydroxysuccinimide (NHS) and tris ($\geq 99.8\%$) were purchased from ThermoFisher Scientific (Waltham, MA, USA).



- When writing, it's a good idea to include the last comma before the **and**.
- The comma is optional after a short introductory adverbial phrase unless the comma is required for clarity.

e.g.,

Either: In recent years, the delta function has been rigorously defined.

Or: In recent years the delta function has been rigorously defined.



A comma follows, but does not precede, restrictive introductory elements:

Wrong

Recombination rate is larger than quenching rate, and, after lasing is achieved, both are smaller than photo dissociation rate.

Correct

Recombination rate is larger than quenching rate, and after lasing is achieved, both are smaller than photo dissociation rate.



Wrong

The laser pulse was reasonably stationary, although, at 1.6 msec, motion of the arc is evident.

Correct

The laser pulse was reasonably stationary, although at 1.6 msec, motion of the arc is evident.

Exception:

Correct Note that, even though they are unbounded, the delta functions are plotted as arrows with their heights representing the coefficient magnitudes



- Enclose parenthetical expressions between commas

e.g., The best way to learn chemistry, unless you are limited by resources, is to perform related experiments yourself.

- A name or title in direct address is parenthetical.

e.g.,

a. If, Sir, you refuse, I cannot predict what will happen.

b. Well, Susan, this is a fine mess you are in.



► Use a comma before, but not after, the coordinating conjunctions “and”, “or”, “nor”, “but”, “yet”, “for”, and “so” connecting two or more main clauses (complete thoughts).

- a. Toluene and hexane were purified by standard procedures, and benzene was redistilled from calcium hydride.
- b. The role of organic templates in zeolite synthesis has been studied extensively, but no general principles have been delineated.
- c. Supported metals are among the most important industrial catalysts, yet only a few have been studied thoroughly.



► Use a comma after a subordinate clause that precedes the main clause in a complex sentence.

- a. Although 40 different P450 enzymes have been identified, only six are responsible for the processing of carcinogens.
- b. Since the institute opened, plant breeders have developed three new prototypes.
- c. Because the gene and the molecular marker are so close on the chromosome, they segregate together in the progeny.



► Use a comma after most introductory words and phrases.

However, the public is being inundated with stories about cancer-causing chemicals.

Therefore, the type of organic solvent used is an important factor in lipase-catalyzed enzymatic synthesis.

After 3 months, the plants grown under phosphorus-deficient conditions were evaluated.

Thus, their motion is the result of the rotation of ferromagnetic domains.



► In compound sentences containing coordinating conjunctions, the clause following the conjunction is punctuated as if it were alone.

- a. The reaction proceeds smoothly, and by use of appropriate reagents, the yields will be enhanced.
- b. The compounds were separated, and after the filters had been washed, the experiments were completed.



► Do not use a comma to separate a verb from its subject, its object, or its predicate noun.

Incorrect

The addition of substituted silanes to carbon-carbon double bonds, has been studied extensively.

Correct

The addition of substituted silanes to carbon-carbon double bonds has been studied extensively.



Incorrect: The disciplines described in the brochure include, materials science, biotechnology, and environmental chemistry.

Correct: The disciplines described in the brochure include materials science, biotechnology, and environmental chemistry.

Incorrect: The solvents used in this study were, cyclohexane, methanol, *n*-pentane, and toluene.

Correct: The solvents used in this study were cyclohexane, methanol, *n*-pentane, and toluene.



► Do not use a comma before the conjunction joining a compound predicate consisting of only two parts.

Incorrect

The product distribution results were obtained in sodium hydroxide, and are listed in Table 10.

Correct

The product distribution results were obtained in sodium hydroxide and are listed in Table 10.



► Use commas to separate items in a series that contains another series in parentheses already separated by commas.

The structure was confirmed with spectroscopy (¹H NMR, UV, and IR), high-resolution mass spectrometry, and elemental analysis.



► Use a comma between two or more adjectives preceding a noun only if you can reverse the order of the adjectives without losing meaning. If you can insert the word “and”, the comma is correct.

- a. The intense, broad signals of the two groups confirmed their location. The broad, intense signals of the two groups confirmed their location.
- b. Sample preparation is a repetitious, labor-intensive task. Sample preparation is a labor-intensive, repetitious task.



But:

- a. Polyethylene is an important industrial polymer.
- b. The rapid intramolecular reaction course leads to ring formation.
- c. The backbone dihedral angles were characterized by *J* couplings.
- d. The local structural environment of the Mn cluster was determined.



► Use a comma before, but not after, the subordinating conjunction in a non re-strictive clause.

Incorrect

The bryopyran ring system is a unique requirement for anticancer activity **whereas**, the ester substituents influence the degree of cytotoxicity.

Correct

The bryopyran ring system is a unique requirement for anticancer activity, **whereas** the ester substituents influence the degree of cytotoxicity.



► Use commas to set off nonrestrictive phrases or clauses.

The products, **which were produced at high temperatures**, were unstable.



► Phrases introduced by “such as” or “including” can be restrictive (and thus not set off by commas) or nonrestrictive (and thus set off by commas).

Potassium compounds **such as KCl** are strong electrolytes; other potassium compounds are weak electrolytes.

Divalent metal ions, **such as** magnesium(II) and zinc(II), are located in the catalytic active sites of the enzymes.

Hydrogen-bonded complexes, **including** proton-bound dimers, are well-known species.



► An appositive is a noun that follows another noun and identifies or explains the meaning of the first noun.

a. My wife, Jeanne, is a biochemist at the National Institutes of Health.

b. My son James plays baseball, and my son John plays soccer.

An appositive is nonrestrictive when **it names the only possibility**. In the first sentence, Jeanne is a nonrestrictive appositive. An appositive is restrictive when it points out one of two or more possibilities.



► Use commas to set off the words “that is”, “namely”, and “for example” when they are followed by a word or list of words and not a clause. Also use a comma after the item or items being named. Use a comma after “i.e.” and “e.g.” in parenthetical expressions.

a. The new derivatives obtained with the simpler procedure, **that is**, reaction with organocuprates, were evaluated for antitumor activity.

b. Alkali metal derivatives of organic compounds exist as aggregates of ion pairs, **namely**, dimers, trimers, and tetramers, in solvents of low polarity.

c. Many antibiotics, **for example**, penicillins, cephalosporins, and vancomycin, interfere with bacterial peptidoglycan construction.

d. These oxides are more stable in organic solvents (**e.g.**, ketones, esters, and ethers) than previously believed.



► Use commas to separate two reference citation numbers, but use an en dash (–) to express a range of three or more in sequence, whether they are superscripts or are on the line in parentheses. When they are superscripts, do not use a space after the comma.

Experimental investigations^{10,14,18–25} concerned the relative importance of field and electronegativity effects.

Certain complexes of cobalt were reported (10, 11) to have catalytic effects on hydrolysis reactions.

Flash photolysis studies (3–7) demonstrated the formation of transient intermediate products such as triplet states.



► Use a comma before Jr. and Sr., but treat II and III according to the person's preference. Within a sentence, always use a comma after Jr. and Sr., but use a comma after II and III only if they are preceded by a comma.

- a. William M. Delaney, Jr.
- b. Charles J. Smith, III
- c. John J. Alden II
- d. William M. Delaney, Jr., was elected to the governing board.
- e. Charles J. Smith, III, received a majority of the votes.
- f. John J. Alden II did not run for office this year.



► Do not use a comma preceding “et al.” unless commas are needed for other reasons.

- Saltzman et al.
- Saltzman, M. J., et al.
- Saltzman, Brown, et al.



► In dates, use a comma after the day, but not after the month when the day is not given.

June 15, 1996
June 1996

► When giving a complete date within a sentence, use a comma after the year as well.

On August 18, 1984, an extraordinary person was born.



► When a geographical location is named within a sentence and the name includes a comma, use a comma at the end of the name as well.

- a. The University of Southern Mississippi, Hattiesburg, MS, USA, is my current employer.
- b. The lead researcher, who obtained her education at the Beijing University of Technology, Beijing, China, addressed the reporters' questions.



► Use a comma to introduce quotations.

In the words of Pasteur, "Chance favors the prepared mind." Pasteur said, "Chance favors the prepared mind."

► Do not use a comma after a quotation that is the subject of the sentence.

"Chance favors the prepared mind" is a translation from the French. (The quotation is the subject of the sentence.)



Period

► Use a period at the end of a declarative sentence, but ***never*** in combination with any other punctuation marks.

- a. He said, "Watch out!"
- b. She asked, "May I go?"

► Do not use periods after most abbreviated units of measure, except when the abbreviation could be confused with a word (**in.** for inches, **at.** for atomic, **no.** for number).



► If a sentence ends with an abbreviation that includes a period, **do not** add another period.

She will return at 3 a.m.

► Use periods and spaces after initials in persons' names.

J.-L. Gay Lussac J. E. Lennard-Jones M. S. Newman

Exception Use periods but no spaces when referring to authors of a paper in the acknowledgment paragraph.

R.C.McD. and C.R. thank Dr. Rose Allan for carefully reading the manuscript.



► Do not use periods in abbreviations or acronyms of institution or organization names.

ACS
CNRS
NASA
NIH
NSF
USM



Semicolon

► Use a semicolon to separate independent clauses that are not joined by a con-junction.

All solvents were distilled from an appropriate drying agent; tetrahydrofuran and diethyl ether were also pretreated with activity I alumina.

(here “;” can be replaced with “, and”)



► Use semicolons between items in a series of words, phrases, or data strings if one or more of the items already contain commas.

- We thank Zachary Axelrod, University of Michigan, for spectral data; Caroline Fleissner, Harvard University, for helpful discussions; and the National Science Foundation for financial support (Grant XYZ 123456).
- Figure 1. Cyclic voltammograms in dichloromethane: (a) compound 1, 23 °C; (b) compound 2, -40 °C; (c) compound 4, 23 °C.
- Figure 6. Ru-H stretches in the IR spectrum of compound 5: ×, 298 K; +, 90 K.



► The above rule holds even if the only group containing the commas is the last in the series.

e.g.,

The compounds studied were methyl ethyl ketone; sodium benzoate; and acetic, benzoic, and cinnamic acids.



► Use a semicolon between independent clauses joined by conjunctive adverbs or transitional phrases such as “that is”, “however”, “therefore”, “hence”, “indeed”, “accordingly”, “besides”, and “thus”.

The rate at which bleaching occurred was dependent on cluster size; **that is**, the degradation of the mononuclear cluster was about 5 times faster than that of the tetranuclear cluster.

Many kinetic models have been investigated; **however**, the first-order reactions were studied most extensively.



- The proposed intermediate is not easily accessible; **therefore**, the final product is observed initially.
- The restriction of the rotational motions of the *tert*-butyl group gives rise to large entropy changes for the association reaction; **hence**, the covalent form is relatively easy to identify.
- The efficiency of the cross-coupling depends on the nature of X in RX; **thus**, the reaction is performed at room temperature by slow addition of the ester.



► Do not use a semicolon between dependent and independent clauses.

Incorrect

The activity on bromopyruvate was decreased; whereas, the activity on pyruvate was enhanced.

Correct

The activity on bromopyruvate was decreased, whereas the activity on pyruvate was enhanced.



Colon

► Use a colon to introduce a word, a phrase, a complete sentence, or several complete sentences that illustrate, clarify, or expand the information that precedes it. Capitalize the first word after a colon **only if** the colon introduces more than one complete sentence, a quotation, or a formal statement.



- The electron density was studied for the ground state of three groups of molecules: (1) methane–methanol–carbon dioxide, (2) water–hydrogen peroxide, **and** (3) ferrous oxide–ferric oxide.
- We now report a preliminary finding: no chemical shift changes were detected in the concentration range 0.1–10 M.
- The following are our conclusions: **L**arge-angle X-ray scattering studies give us an accurate picture of structures up to 9 Å. They do not allow the specification of defects, such as random ruptures of the chains. The structural models defined are strongly supported by magnetic measurements.



► In figure captions, use a colon to introduce explanations of symbols or other aspects of the figure.

- Figure 1. Variable-temperature ^1H NMR spectra of compound **12**: top, 403 K; middle, 353 K; bottom, 298 K.
- Figure 3. Brønsted-type plots for aminolysis in 1 M KCl at 25 °C: □, 2-nitrophenyl acetate; △, 3-chlorobenzoic acid; Δ, 2,6-dinitrobenzoic acid.



► Do not use a colon (or any punctuation) between a verb and its object or complement or between a preposition and its object.

Incorrect

The rate constants for the reaction in increasing concentrations of sodium hydroxide are: 3.9, 4.1, 4.4, 4.6, and 4.9.

Correct

The rate constants for the reaction in increasing concentrations of sodium hydroxide are 3.9, 4.1, 4.4, 4.6, and 4.9.



Incorrect: The thermal decomposition was investigated with: gas chromatography, BET surface areas, and X-ray powder diffraction.

Correct: The thermal decomposition was investigated with gas chromatography, BET surface areas, and X-ray powder diffraction.

Incorrect: Transition-metal nitrides have many properties that make them suitable for industrial applications, including: high wear resistance, high decomposition temperature, and high microhardness.

Correct: Transition-metal nitrides have many properties that make them suitable for industrial applications, including high wear resistance, high decomposition temperature, and high microhardness.



► Use either a colon or a slash to represent a ratio, but not an en dash. Use either a slash or an en dash between components of a mixture, but not a colon.

dissolved in 5:1 glycerin/water

dissolved in 5:1 glycerin–water

the metal/ligand (1:1) reaction mixture

the metal–ligand (1:1) reaction mixture

the metal–ligand (1/1) reaction mixture

the methane/oxygen/argon (1/50/450) matrix

the methane/oxygen/argon (1:50:450) matrix



Quotation marks

► In ACS style, *which may differ from other authorities*, location of closing quotation marks follow logical placement.

- a. if the punctuation is part of the quotation, then it should be within the quotation marks.
- b. if the punctuation is not part of the quotation, the writer should not mislead the reader by implying that it is.



► Place closing quotation marks before all punctuation that is not part of the original quotation. Place them after all punctuation that is part of the quotation.

- a. The sample solution was stirred briefly with a magnetic “flea”.
- b. Ralph Waldo Emerson said, “The reward of a thing well done is to have done it.”



► Use quotation marks around words used in a new sense or words not used literally, but only the first time they appear in text.

- a. Plastocyanin is a soluble “blue” copper protein.
- b. The integrated intensity of each diagonal in the spectrum is proportional to a “mixing coefficient”.
- c. The “electron-deficient” cations are, in fact, well-established intermediates.



► Use quotation marks to enclose the titles of uniquely named parts and sections of a book or a paper.

A complete description of the oils is given in the section “Flavonoids in Citrus Peel Oils”, and other references are listed in the bibliography.

But:

The preface describes the complexity of the problem.



► Use quotation marks to enclose short direct quotations (up to **three sentences**).

In the book *Megatrends*, Naisbitt concludes, “We are moving from the specialist who is soon obsolete to the generalist who can adapt.”



► Use a narrower column width (that is, indented on both sides) for longer quotations (extracts) of 50 words or more. **Do not** use quotation marks.

Everything is made of atoms. That is the key hypothesis. The most important hypothesis in all of biology, for example, is that everything that animals do, atoms do. In other words, there is nothing that living things do that cannot be understood from the point of view that they are made of atoms acting according to the laws of physics.

—Richard Phillips Feynman



Exception: in interview

However, the above convention does not apply in an article quoting someone who has been interviewed. In such cases, quoted text need not be differentiated by column width, and quotation marks should be used.



Single vs double quotation marks

► Use single quotation marks only when they are within double quotation marks.

He said, "You should read the article 'Fullerenes Gain Nobel Stature' in **the** January 6, 1997, issue of *Chemical & Engineering News*."



Parentheses ()

Parenthetical expressions contain information that is subsidiary to the point of the sentence. The sentence does not depend on the information within the parentheses.



► Use parentheses for parenthetical expressions that clarify, identify, or illustrate and that direct the reader.

- a. The total amount (10 mg) was recovered by modification of the procedure.
- b. The final step (washing) also was performed under a hood.
- c. The curve (Figure 2) obeys the Beer–Lambert law.
- d. The results (Table 1) were consistently positive.
- e. Only 15 samples (or 20%) were analyzed.



► Punctuate after, not before, parenthetical expressions.

Incorrect

Compound **1**, (7 mg) obtained by typical workup methods, was used without further purification.

Correct

Compound **1** (7 mg), obtained by typical workup methods, was used without further purification.



► If a parenthetical sentence is within another sentence, do not use a final period within the closing parenthesis, and do not start the parenthetical sentence with a capital letter.

Our results (the spectra are shown in Figure 5) justified our conclusions. Our results justified our conclusions (the spectra are shown in Figure 5).



► If a parenthetical **sentence is not** within another sentence, use a final period inside the closing parenthesis, and start the parenthetical sentence with a capital letter.

A mechanism involving loss of a CH radical followed by rearrangement was proposed. (The reactions are shown in Scheme 1.)



► Use parentheses to enclose numerals in a list. Always use parentheses in pairs, not singly.

Three applications of this reaction are possible: (1) isomerization of sterically hindered aryl radicals, (2) enolketo transformation, and (3) sigmatropic hydrogen shift.



► Use parentheses to identify the manufacturer of reagents and equipment.

cobalt chloride (Mallinckrodt)
a pH meter with a glass electrode (Corning)

► Do not use parentheses when citing a reference number in narrative text. In such a case, the reference number is the point of the sentence, not subsidiary information, and thus not parenthetical.

Incorrect: in ref (12), in (12)

Correct: in ref 12



Square brackets []

► Use square brackets within quotation marks to indicate material that is not part of a direct quote.

In the words of Sir William Lawrence Bragg, “The important thing in science is not so much to obtain new facts as to *discover new ways* [italics added] of thinking about them.”

► Use square brackets to indicate concentration: $[Ca^{2+}]$.



► Use square brackets to indicate concentration: $[Ca^{2+}]$.

► Use square brackets in mathematical expressions as discussed in Chapter 11 and in chemical nomenclature and notation as discussed in Chapters 12 and 13.



Dashes

The shortest dash is the hyphen (-); the en dash (–) is longer; and the em dash (—) is the longest.



► Hyphen – used to connect words and parts
Hyphens are sometimes used to connect a prefix to a word. The tendency is to eliminate the hyphen after a prefix.

quasi-reversible (quasireversible)
micro-electrodes (microelectrode)
electroreduction (electroreduction)



► Hyphenate a word that might be misread or difficult to read without the hyphen (e.g., when letters are doubled; when more than one prefix is present; and when the unhyphenated form does not convey the intended meaning.)

un-uniform
co-ion
sub-subcommittee

micro-organism
anti-inflation
electro-oxidation



► Do not hyphenate a number and a unit of time or measure used as a unit modifier.

$1.2 \times 10^{-4} \text{ cm}^{-1}$ peak
25 K increments
10 mg sample (not 10-mg sample)
a 0.1 mol dm^{-3} solution
20 mL aliquot
 12° angle



► When two or more unit modifiers with the same ending base modify one noun, use a hyphen after each element, and do not repeat the ending base.

first- and second-order reactions
high-, medium-, and low-frequency measurements

► Do not hyphenate unit modifiers that are chemical names.

acetic anhydride concentration
amino acid level
barium sulfate precipitate
sodium hydroxide solution



En Dash

► Use an en dash to mean the equivalent of “and”, “to”, or “versus” in multiword concepts where the words are of equal weight.

acid–base titration	bromine–olefin complex
carbon–oxygen bond	cis–trans isomerization
cost–benefit analysis	dose–response relationship
ethanol–ether mixture	freeze–pump–thaw
degassed helix–coil transition	host–guest complexation



► Use an en dash to mean “to” or “through” with a span of three or more numerals or other types of ranges.

12–20 months	Figures 1–4	5–50 kg
Sections 1b–1f	parts C–E	
Compounds A–I		



exception 1 When either one or both numbers are negative or include a symbol that modifies the number, use the word “to” or “through”, not the en dash.

–20 to +120 K –145 to –30 °C ≈50 to 60
10 to >600 mL <5 to 15 mg

exception 2 Do not use an en dash when the word “from” or “between” is used.

from 500 to 600 mL (*not* from 500–600 mL)
between 7 and 10 days (*not* between 7–10 days)



► Use an en dash to link the names of two or more persons of equal importance used as a modifier.

Bednorz–Müller theory Beer–Lambert law
Bose–Einstein statistics Debye–Hückel theory
Diels–Alder reaction Fermi–Dirac statistics
Flory–Huggins interaction Franck–Condon factor
Geiger–Müller effect
Henderson–Hasselbalch equation
Jahn–Teller effect



Em Dash

► Use em dashes to set off words that would be misunderstood without them.

Incorrect

All three experimental parameters, temperature, time, and concentration, were strictly followed.

Correct

All three experimental parameters—temperature, time, and concentration—were strictly followed.



► Do not use em dashes to separate phrases or nonrestrictive clauses if another form of punctuation can be used.

Incorrect: Knauth—not Stevens—obtained good correlation of results and calculations.

Correct: Knauth, not Stevens, obtained good correlation of results and calculations.

Incorrect: The singly charged complexes—which constituted bands 1 and 3—liberated maleate anion upon decomposition.

Correct: The singly charged complexes, which constituted bands 1 and 3, liberated maleate anion upon decomposition.



Ellipsis points ...

► Within a quotation, use three periods (points of ellipsis) to indicate deleted words or phrases. These three periods are in addition to other needed punctuation. Thus, if a period is already there, the result will be four periods.

No science is immune to the infection of politics and the corruption of power.... The time has come to consider how we might bring about a separation, as complete as possible, between Science and Government in all countries.

—Jacob Bronowski



► Do not begin or end a quotation with ellipsis points.

► Use ellipsis points where part of a series is omitted, when the pattern of the series is unambiguous.

$a = 1, 2, 3, \dots$


$n = 2, 4, 6, \dots$

$x = 1, 3, 5, \dots, 15$



Special Typefaces

- ▶ Italic Type
- ▶ Greek letters
- ▶ Capitalizations




- ▶ Use italic type sparingly to emphasize a word or phrase. Do not use italics for long passages.

- For emphasis

Oxidation is a process in which an atom *loses* an electron.


Absorption is light *absorbed* by an analyte of interest, whereas emission is light *emitted* by a species after light is absorbed.



- ▶ Use italic type for a word being defined or for a newly introduced term the first time it appears in text.

In an *outer-sphere transfer*, an electron moves from reductant to oxidant with no chemical alteration of the primary coordination spheres.

We call these materials *microcapsules*.



Italics for symbology

► Most mathematical symbols and letter symbols representing a physical concept are italic, whether within roman or italic text.

Beer's law $A = \epsilon bc$

$I = V/R$

$E = 1.20 \text{ V vs Ag/AgCl}$

Figure X- & Y-axis labels

$[i_{CV} \text{ (mA) vs } E \text{ (V)}]$



► Do not use italic type for "pH"; "p" is always lowercase, and "H" is always capitalized.

► Do not use italic type for M (molar) or N (normal). Do use italic type for m (molal).

pH
 pK_a



► Use italic type for

- variables: T for temperature, x for mole fraction, r for rate
- axes: the y axis
- planes: plane P
- components of vectors and tensors: $a_1 + b_1$
- elements of determinants and matrices: g_n
- constants: k_B , the Boltzmann constant; g , the acceleration due to gravity
- functions that describe variables: $f(x)$



Greek Letters

► Use Greek letters, not the spelled-out words, for chemical and physical terms. Do not italicize Greek letters.

- α helix (*not* alpha helix)
- β particle (*not* beta particle)
- β sheet (*not* beta sheet)
- γ radiation (*not* gamma radiation)
- NF κ B (nuclear factor κ B) (*not* NF kappa B)

exceptions

- delta opioid receptor
- mu opioid receptor



Capitalization

► Capitalize the first letter of the names of programs, and follow the manufacturer's or creator's usage within the name.

- Acrobat
- ChemDraw
- EndNote
- HyperChem
- ISIS/Draw
- MathType
- Microsoft Excel



► Capitalize the words "figure", "table", "chart", and "scheme" only when they refer to a specific numbered item.

- Chart 4 Schemes 4–7
- Figure 1 Table II

► Do not capitalize the "r" in "X-ray" at the beginning of a sentence or in a title.

► Do not capitalize the names of the four seasons: summer, fall, autumn, winter, spring.



► Capitalize parts of a book when they refer to a specific titled and numbered part.

Appendix I
Chapter 3
Section 4.2

But

the appendix
the chapter
the contents
the preface



► When a sentence begins with a symbol that is not hyphenated to the following word, the word is not capitalized.

π -Electron contributions are evident.
 π electrons make significant contributions in this system.
 σ values were calculated from eq 3.



► Do not capitalize the word “**model**” with a number or code.

- a. γ counter (Beckman model 5500B)
- b. mass spectrometer (PerkinElmer model 240C)
- c. multichannel spectrometer (Otsuka model MCPD-1000)
- d. spectrometer (Varian model XL-200)
- e. Waters model 660 gradient controller



► In titles and headings, capitalize the main words (nouns, pronouns, verbs, adjectives, adverbs, and subordinating conjunctions) regardless of the number of letters.

► Do not capitalize coordinating conjunctions (“and”, “but”, “or”, “nor”, “yet”, “so”), articles (“a”, “an”, “the”), or prepositions.

► Do capitalize the “to” in infinitives. Do capitalize the first and last words of a title or heading, regardless of part of speech, unless the word is mandated to be lowercase (e.g., pH, d Orbital).



Exception 1: In titles and headings, capitalize small words that are parts of phrasal verbs.

Break Down Build Up Set Off
Set Up Slow Down Wear Out

Exception 2: In titles and headings, capitalize small words that are parts of phrasal adjectives.

End-On Bonding
In-Plane Atoms
Side-On Bonding
(*but* Out-of-Plane Vibrations)



► Capitalize parenthetical phrases in titles and headings as if they were not parenthetical.

Versatile Organic (Fullerene)–Inorganic (CdTe Nanoparticle) Nanoensembles



Numbers

► With items other than units of time or measure, use words for cardinal numbers less than 10; use numerals for 10 and above. Spell out ordinals “first” through “ninth”; use numerals for 10th or greater.

three flasks	30 flasks	third flask
12 th flask	seven trees	10 trees
eighth example	33 rd example	first century
21 st century	sixfold	20-fold



Exception 1: Use all numerals in a series or range containing numbers 10 or greater, even in nontechnical text. e.g., (a) 5, 8, and 12 experiments, (b) 5–15 repetitions

Exception 2: Use all numerals for numbers modifying nouns in parallel construction in the same sentence if one of the numbers is 10 or greater. e.g., Activity was reduced in 2 pairs, not significantly changed in 11 pairs, and increased in 6 pairs.

Exception 3: For very large numbers used in a nontechnical sense, use a combination of numerals and words. e.g., (a) 1 billion tons, (b) 180 million people, (c) 2 million pounds (*not* lb), (d) 4.5 billion years, and (e) \$15 million (*not* 15 million dollars)



► Use words and unit of measure to begin a sentence.

- Twelve species were evaluated in this study.
- Twenty-five milliliters of acetone was added, and the mixture was centrifuged.

However, if possible, recast the sentence.

Acetone (25 mL) was added, and the mixture was centrifuged.

A 25 mL portion of acetone was added, and the mixture was centrifuged.



► Even when a sentence starts with a spelled-out quantity, use numerals when appropriate in the rest of the sentence.

- a. Twenty-five milliliters of acetone and 5 mL of HCl were added.
- b. Three micrograms of sample was dissolved in 20 mL of acid.
- c. Fifty samples were collected, but only 22 were tested.



► When the suffix “fold” is used in a *nonmathematical sense*, spell out the accompanying number if it is less than 10.

The purpose of this discussion is twofold.

► When the word “times” is used in a nonmathematical sense, spell out the accompanying number if it is less than 10.

The beaker was rinsed four times.



► Use numerals for expressions used in a *mathematical sense*.

- a. The incidence of disease increased by a factor of 4.
- b. The yield of product was decreased by 6 orders of magnitude.
- c. The efficiency of the reaction was increased 2-fold.
- d. After 2 half-lives, the daughter product could be measured.
- e. The control group had 3 times the risk for colon cancer.
- f. The values are determined with 5 degrees of freedom.



► Use numerals in ratios.

a ratio of 1:10

a ratio of 1/10

a 1:1 (v/v) mixture

a 1/1 (v/v) mixture

No space before and after “:” or “/”



► In dates, use numerals without ordinal endings.

a. January 3, Jan 3 (*not* January 3rd, Jan 3rd)

b. September 5, Sept 5 (*not* September 5th, Sept 5th)

► Use numerals for decades, and form their plurals by adding an “s”. Do not use apostrophes in any position.

a. the 1960s (*not* the 1960’s, *not* the ’60s)

b. values in the 90s (*not* the 90’s)

c. She is in her 20s. (*not* her 20’s)



Scientific Writing

IV. Word Usage, Sentences, and Paragraphs

Dr. Wujian Miao



Tricky Possessives

▶ Form the possessive of a joint owner by adding an apostrophe and an "s" after the last name only.

- a. Celapino and Marshall's results
- b. Bausch and Lomb's equipment

▶ Form the possessive of plural nouns that do not end in "s" by adding an apostrophe and an "s" ..

- a. people's rights
- b. children's book



▶ Form the possessive of plural nouns that end in "s" by adding an apostrophe only.

compounds' structures

▶ Form the possessive of a proper name ending in "s" by adding an apostrophe and an "s".

- a. Jacobs's laboratory
- b. Mathers's reception



Tricky Plurals

Singular	plural (preferred forms first)
alga	algae
apparatus	apparatus, apparatuses
appendix	appendixes, appendices
bacterium	bacteria
basis	bases
criterion	criteria, criterions
erratum	errata
fungus	fungi, funguses
helix	helixes, helices
hypothesis	hypotheses
index	indexes



maximum	maximums, maxima
medium	media, mediums
minimum	minimums, minima
phenomenon	phenomena, phenomenon
polyhedron	polyhedrons, polyhedra
spectrum	spectra, spectrums
symposium	symposia, symposiums
vertex	vertexes, vertices



Recommended spelling list

Absorbance	air-dry (verb)	ambiguous
amine (RNH ₂)	ammine (NH ₃ complex)	
analog (computer)	analogue (structural derivative)	
Analyte	analyze	antioxidant
Appendixes	aqua regia	asymmetry
autoxidation	auxiliary	back-titrate (verb)
break up (verb)	breakup (noun)	
broad band (noun)	broad-band (adjective)	
build up (verb)	buildup (noun)	



canceled cannot catalog
clean up (verb) cleanup (noun)
close up (verb) close-up (noun)
co-ion co-occurrence co-worker
coauthor collinear colorimetric
counter electrode counteranion counterion
cross-coupling cross-link
cross over (verb) crossover (noun, adjective)
cross section (noun) cross-sectional (adjective)
cut off (verb) cutoff (noun) cuvette
desiccator dry ice drybox electroless
fall off (verb) falloff (noun, adjective)



far-infrared faradic (referring to current, not the person)
fax (noun, verb, adjective)
fiber-optic (adjective) fiber optics (noun)
follow up (verb) follow-up (noun, adjective)
glovebag glovebox
heat-treat (verb) hemoglobin
heterogeneous homogeneous
ice-cold ice-water bath (use en dash)
isopropyl alcohol (*not* isopropanol)
lifetime line shape line width
make up (verb) makeup (noun)
mid-infrared midpoint



Monochromator near-ultraviolet Nernstian
occurred occurrence occurring
path length
re-form (to form again) reform (to amend)
scale up (verb) scale-up (noun)
Seawater self-consistent selfsame
set up (verb) setup (noun)
steam-distill (verb) ultrahigh vacuum
voltmeter (measures voltaic electricity)
voltammeter (measures ranges of volts and amperes)
work up (verb) workup (noun)



Correct sentence structure

Verb voice and tense

► Simple past tense is correct for stating what was done, either by others or by you.

- The solutions **were heated** to boiling.
- We **found** that relativistic effects enhance the bond strength.
- The structures **were determined** by neutron diffraction methods.



► Present tense is correct for statements of fact.

- Absolute rate constants for a wide variety of reactions **are** available.
- Hyperbranched compounds **are** macro-molecular compounds that **contain** a branching point in each structural repeat unit.



Past tense and present perfect

- was** → history (no connection with the present)
has been → recent and perhaps ongoing

Examples of misuse of present perfect (with corrections):

At the same time it ~~has been~~^{was} shown...
These studies ~~have~~ acquired new impetus...
The way out of this difficulty ~~has been~~^{was} indicated by...

Examples of correctly used present perfect:

In this section we ^{have} ^ tried to...
Recent research ^{has} ^ focused on...



Other Forms

► It is acceptable to use split infinitives to avoid awkwardness or ambiguity.

- Awkward

The program is designed to **assist financially** the student who is considering a career in chemistry.

- Better

The program is designed to **financially assist** the student who is considering a career in chemistry.



Ambiguous

The bonded phases allowed us to **investigate fully** permanent gases.

Better

The bonded phases allowed us to **fully investigate** permanent gases.



Placements of adverbs

❶ Place adverbs before the verb!

Wrong: Impurities affect **also** the elastic properties.

Right: Impurities **also** affect the elastic properties.

Wrong: If we extend **further** the analogy...

Right: If we **further** extend the analogy...

❷ ... or between the auxiliary and the verb!

will **rapidly** converge

has **long** been known

could **severely** limit

can **no longer** be seen

would **then** follow

had **not yet** received



Place the verb early in the sentence!

very poor!

If the processes of entropy generation such as plasma heating owing to decay or the annihilation of massive particles when they depart from thermal equilibrium are neglected, then...

much better!

If ^{we neglect} [^] the processes of entropy generation such as plasma heating owing to decay or the annihilation of massive particles when they depart from thermal equilibrium ~~are neglected~~, then...



Subjects and subject-verb agreement

► Use first person when it helps to keep your meaning clear and to express a purpose or a decision.

Jones reported xyz, but **I (or we)** found

I (or we) present here a detailed study

My (or our) recent work demonstrated

To determine the effects of structure on photophysics, **I (or we)**



However, avoid clauses such as

“we believe”,

“we feel”, and

“we can see”, as well as personal opinions.



► The number of the subject can be obscured when one or more prepositional phrases come between the subject and the verb.

Application of this technique to studies on the phytoplankton biomass and its environments **is described**. (The subject is “application”, which is singular.)

► The number of the subject can be obscured when the sentence is constructed in the order prepositional phrase, verb, subject.

To the mixture **were added** KCl, HEPES, and water. To the solution **was added** the parent compound.



► Two singular subjects joined by “and” require a plural verb.

Growth **and** isolation of M13 virus **were described**.

Exception: A subject that is plural in form but singular in effect takes a singular verb. Here a compound subject functions as a single entity.

- a. Research and development is attracting a growing number of young scientists. Its inventor and chief practitioner is a native son of Boston, Robert Coles.
- b. Much inconsistency and confusion exists with technical documentation.



► When two or more subjects are joined by “or”, the verb takes the number of the closer or closest subject.

- a. All of the pH values or the median pH value was used.
- b. The median pH value or all of the pH values were used.



► Collective nouns take a singular verb when the group as a whole is meant; in that case, they are often preceded by the word “the”. Collective nouns take a plural verb when individuals of the group are meant; in that case, they are often preceded by the word “a”.

contents	majority	range
couple	number	series
dozen	pair	variety
group		



- The number of metal amides synthesized was the largest to date. (Refers to the number as a unit.)
- A number of metal amides were synthesized. (Refers to each amide.)
- The series of compounds was prepared to test the hypothesis. (Refers to the series as a unit.)
- A series of compounds were tested. (Refers to each compound.)



- The variety of materials tested was sufficient for comparative analysis. (Refers to variety as a unit.)
- A variety of materials were tested for selective removal of ^{90}Sr from nuclear waste solutions. (Refers to the materials individually.)
- This group of workers is well aware of its responsibilities. (Refers to the group as a unit.)
- This group of workers are willing to sign their names. (Refers to the individuals.)



► “Data” can be a singular or plural noun.

- a. After the data is printed and distributed, we can meet to discuss it. (Refers to the whole collection of data as one unit.)
- b. Experimental data that we obtained are compared with previously reported results. (Refers to the data as individual results.)



► Units of measure are treated as collective nouns that take a singular verb.

- a. The mixture was stirred, and 5 mL of diluent **was** added. **Five grams** of NaCl **was** added to the solution.
- b. **Three weeks** **is** needed to complete the experiment.
- c. To the mixture **was** added **5 g** of compound **B**.
- d. Under high pressure, **5 volumes** of solution A **was** added.



► Nouns ending in “ics” and denoting a scientific discipline are usually singular.

dynamics mechanics
kinetics physics
mathematics thermodynamics

- a. Mechanics involves the application of Newton’s three laws of motion.
- b. The kinetics of electron transfer to and from photogenerated radicals was examined by laser flash photolysis.
- c. The thermodynamics is governed by the positions of the valence and conduction bands.



► Compound subjects containing the words “each”, “every”, and “everybody” take singular verbs.

- a. Each flask and each holder was sterilized before use.
- b. Every rat injected and every rat dosed orally was included.
- c. Everybody in the group and every visitor is assigned a different journal each month.

► Sometimes, one of these words is implicit; such cases take a singular verb.

Each name and address is entered into the database.



► If both components of the compound subject do not contain, explicitly or implicitly, one of the words “each”, “every”, or “everybody”, the verb must be plural.

Each student and all the professors were invited.



► Indefinite pronouns themselves (or adjectives combined with the indefinite pronoun “one”) can be the subject of the sentence.

- . Those that take a singular verb are “each”, “either”, “neither”, “no one”, “every one”, “anyone”, “someone”, “everyone”, “anybody”, “somebody”, and “everybody”.
- a. Each was evaluated for its effect on metabolism.
- b. Neither disrupts the cell membrane.
- c. Someone measures the volume every day.



. Those that take a plural verb are “several”, “few”, “both”, and “many”.

- a. Several were evaluated for their effects on metabolism.
- b. Few disrupt the cell membrane.
- c. Regarding compounds 1 and 2, both react with the control agent.
- d. Many were chosen to be part of the study.



. Those that take either a singular or a plural verb, depending on context, are “some”, “any”, “none”, “all”, and “most”. The number of the object of the preposition determines the number of the indefinite pronoun related to it.

- a. All of the money was stolen.
- b. Most of the books were lost.
- c. Not all the disks are here; some were lost.



► When a fraction is the subject of the sentence, the number of the attendant object of the preposition determines the number of the subject.

- a. One-third of the precipitate was dissolved.
- b. One-fourth of the electrons were excited.



► When a subject and its predicate noun disagree in number, the verb takes the number of the subject. (A *predicate noun* is the “complement” of a form of the verb “to be”; it refers to the same person or thing as the subject.)

- a. The preparation and structure determination [plural subject] of these three compounds are the topic [singular predicate noun] of this paper.
- b. The topic of this paper [singular subject] is the preparation and structure determination [plural predicate noun] of these three compounds.



Awkward Omissions of Verbs and Auxiliary Verbs

► Each subject in a compound sentence must have the proper verb and auxiliary verb.

Incorrect

The eluant was added to the column, and the samples collected in 10 mL increments.

Correct

The eluant **was** added to the column, and the samples **were** collected in 10 mL increments.



Sentence modifiers

Modifiers made up of phrases or dependent clauses can be added to simple sentences to indicate, for example, cause and effect, or time sequence, or comparison.

► A *restrictive* phrase or clause is one that is essential to the meaning of the sentence. Restrictive modifiers are not set off by commas.

- a. Only doctoral students who have completed their coursework may apply for this grant.
- b. Several systems that take advantage of this catalysis can be used to create new palladium compounds.



► A *nonrestrictive* phrase or clause is one that adds meaning to the sentence but is not essential; in other words, the meaning of the basic sentence would be the same without it. Nonrestrictive modifiers are set off by commas.

- a. Doctoral students, **who often have completed their coursework**, apply for this teaching fellowship.
- b. Several systems, **which will be discussed below**, take advantage of this catalytic reaction.



► A *misplaced modifier* is one that is placed next to the wrong word in the sentence, so it inadvertently misrepresents the author's intended meaning.

Incorrect

We commenced a new round of experiments unable to point to meaningful conclusions.

Correct



► A *dangling modifier* is one that lacks a word in the sentence to modify in a logical or sensible way.

Incorrect

Adding 2 mL of indicator solution, the end point for the titration was reached.

Correct



► If a modifier precedes the subject of a sentence, it must modify that subject and be separated from it by a comma. Otherwise, it is a dangling modifier.

Incorrect

Splitting the atom, many new elements were discovered by Seaborg.

Correct

[Redacted]



Incorrect

When confronted with these limitations, the experiments were discontinued.

Correct

[Redacted]

Alternative

[Redacted]



Incorrect

Understanding the effect of substituents on the parent molecules, the ortho hydrogens could be assigned to the high-frequency peak.

Correct

[Redacted]



Incorrect

Using the procedure described previously, the partition function can be evaluated.

Correct



► In some cases, the passive voice can be used to correct a dangling modifier.

Incorrect

After combining the reactants, the reaction mixture was stirred at room temperature for 3 h.

Correct



Incorrect

After stirring the mixture, 5 mg of compound **2** was added.

Correct



Sentence construction and word order

► Use an affirmative sentence rather than a double negative.

INSTEAD OF

This reaction is not uncommon.

This transition was not unexpected.

This strategy is not infrequently used.

This result is not unlikely to occur.

CONSIDER USING

This reaction is common.
This reaction is not rare.
This reaction occurs about 40% of the time.

This transition was expected.
We knew that such transitions were possible.

This strategy is frequently used.
This strategy is occasionally used.

This result is likely to occur.
This result is possible.



► Watch the placement of the word “only”. It has different meanings in different places in the sentence.

- Only the largest group was injected with the test compound. (Meaning: and no other group)
- The largest group was only injected with the test compound. (Meaning: and not given the compound in any other way)
- The largest group was injected with only the test compound. (Meaning: and no other compounds)
- The largest group was injected with the only test compound. (Meaning: there were no other test compounds)



► Be sure that the antecedents of pronouns are clear; in other words, when you use a pronoun (for example, “he”, “she”, “it”, or “they”), the noun to which the pronoun refers should be obvious (for example, “Isaac Newton”, “Marie Curie”, “the compound”, or “the research team”). This is particularly true for the pronouns “this” and “that”. If there is a chance of ambiguity, use a noun to clarify your meaning.



Ambiguous

The photochemistry of transition-metal carbonyl complexes has been the focus of many investigations. This is due to the central role that metal carbonyl complexes play in various reactions.

Unambiguous



► Use the proper subordinating conjunctions.

“While” and “since” have strong connotations of time. Do not use them where you mean “although”, “because”, or “whereas”.

Poor

Since solvent reorganization is a potential contributor, the selection of data is very important.

Better

Because solvent reorganization is a potential contributor, the selection of data is very important.



Poor

While the reactions of the anion were solvent-dependent, the corresponding reactions of the substituted derivatives were not.



Parallelism (Equal grammatical rank)

► A *coordinating conjunction* is a single word, such as “and”, “but”, “or”, “nor”, “yet”, “for”, and sometimes “so”.

Incorrect

Compound 12 was prepared analogously and by Lee’s method (5).

Correct



► A *correlative conjunction* is a pairing of words, such as “either ... or”; “neither... nor”; “both ... and”; “not only ... but also”; and “not ... but”.

Incorrect

The product was washed **either** with alcohol **or** acetone.



Incorrect

It is best to use alternative methods **both** because of the condensation reaction **and** because the amount of water in the solvent increases with time.

Correct



Incorrect

Not only was the NiH functionality active toward the C-donor derivatives **but also** toward the N donors.

Correct



► Do not try to use parallel construction around the word “but” when it is not used as a coordinating conjunction.

- a. Increasing the number of fluorine atoms on the adjacent boron atom decreases the chemical shift, but only by a small amount.
- b. The reaction proceeded readily, but with some decomposition of the product.

► Use parallel constructions in series and lists, including section headings and subheadings in text and tables and listings in figure captions.



Not Parallel

Summarizing Project.

Description of Project:

- 1. Giving Background and Stating Objectives
- 2. Design of Research and Methods
- 3. scheduling of project
- 4. Conclusions

List of References

Parallel

- Project Summary
- Project Description
- Background and Objectives
- Research Design and Methods
- Project Schedule
- Conclusions
- References Cited



Comparisons

► Introductory phrases that imply comparisons should refer to the subject of the sentence and be followed by a comma.

Incorrect

Unlike alkali-metal or alkaline-earth-metal cations, hydrolysis of trivalent lanthanides proceeds significantly at this pH.

Correct



Incorrect

In contrast to the bromide anion, there is strong distortion of the free fluoride anion on the vibrational spectroscopy time scale.



Commonly confused words and phrases

Compare to vs Compare with

► Use the verb “compare to” when similarities are being noted. Use “compare with” when differences are being noted. Only things of the same class should be compared.

Compared to compound 3, compound 4 shows an NMR spectrum with corresponding peaks.

Compared with compound 3, compound 4 shows a more complex NMR spectrum.



► Do not omit words needed to complete comparisons (e.g., “than xxx”), and do not use confusing word order.

Incorrect

The alkyne stretching bands for the complexes are all lower than the uncoordinated alkyne ligands.

Correct



Incorrect

The decrease in isomer shift for compound 1 is greater in a given pressure increment than for compound 2.

Correct



Idioms: should not be split

“different from”, “similar to”, “identical to”, “identical with”.

Incorrect: The complex shows a significantly different NMR resonance from that of compound 1.



Incorrect: Compound **5** does not catalyze hydrogenation under similar conditions to compound **6**.



Exception: These idioms can be split if an intervening prepositional phrase modifies the first word in the idiom.



► Phrases such as “relative to”, “as compared to”, and “as compared with” and words such as “versus” are also used to introduce the second element in a comparison. The things being compared must be parallel.

- a. The **greater** acidity of nitric acid **relative to** nitrous acid is due to the initial-state charge distribution in the molecules.
- b. The **lowering** of the vibronic coupling constants for Ni **as compared with** Cu is due to configuration interaction.



Grouping and Comparison Words

► Use “**respectively**” to relate two or more sequences in the same sentence.

The excitation and emission were measured at 360 and 440 nm, respectively.

(That is, the excitation was measured at 360 nm, and the emission was measured at 440 nm.)



More than vs Over

► Use the *more accurate* terms “greater than” or “more than” rather than the *imprecise* “over” or “in excess of”.

- greater than 50% (*not* in excess of 50%)
- more than 100 samples (*not* over 100 samples)
- more than 25 mg (*not* in excess of 25 mg, *not* over 25 mg)



► Do not use “over” to describe relative amounts

More than = greater than
Over = physically above

wrong
She raised over \$500.

Right
She raised more than \$500.



► Use “fewer” to refer to number; use “less” to refer to quantity.

- fewer than 50 animals
- fewer than 100 samples
- less product
- less time
- less work



► However, use “less” with number and unit of measure combinations because they are regarded as singular.

- less than 5 mg
- less than 3 days
- Scan rate was less than 100 mV/s.



Between vs Among

► Use “between” with two named objects; use “among” with three or more named or implied objects.

- a. Communication between scientists and the public is essential.
- b. Communication among scientists, educators, and the public is essential.
- c. Communication among scientists is essential.



I, Myself, and Me

- a. Please give a copy of the agenda to Anne and me, I, or myself?).
- b. I myself checked the agenda.
- c. Cheryl and (I or myself?) checked the agenda.
- d. The agenda was checked by Barbara and (me or myself?).



“Due to” vs “Because of”

“Due to”: adjective (meaning “attributable to”), to modify a noun or pronoun, after “to be”.

“because of”: adverb, to modify verbs

- a. His defeat was **due to** the lottery issue.
- b. He was defeated **because of** the lottery issue.



Cutbacks **due to** decreased funding have left us without basic reference books.

The accuracy of the prediction is **due to** a superior computer program.

~~Due to~~ **Because of** exposure to low level of lead, children can be at risk for developmental problems.



“Based on” vs “On the basis of”

- “based on” must modify a noun or pronoun
- “on the basis of” to modify a verb

a. The doctors’ new methods in brain surgery were **based on** Ben Carson’s work.

b. **On the basis of** the molecular orbital calculations, we propose a mechanism that can account for all the major features of alkali and alkaline earth catalyzed gasification reactions.
(*not* Based on ...)



- a. Our conclusions *are based on* these findings.
- b. Discrimination *based on* disability is illegal as well as unjust.
- c. These guidelines *are based on* our experience.
The movie *is based on* a novel.
- d. He was denied permission *on the basis of* his criminal record.
- e. They have been ranked *on the basis of* their performance.
- f. Entrants compete *on the basis of* speed.



He was hired *on the basis of* his experience.

The plan was decided *on the basis of* our budget.

Stop discrimination *based on* sex.



“Assure”, “Ensure”, and “Insure”

To assure is to affirm; to ensure is to make certain; to insure is to indemnify for money.

- He assured me that the work had been completed.
- The procedure ensures that clear guidelines have been established.
- You cannot get a mortgage unless you insure your home.



“Affect”, “Effect”, and “Impact”

- “affect” (v, to influence, modify, or change)
- “effect” (n, consequence, outcome, or result)
- “impact” (n, a significant effect)

- a. The increased use of pesticides affects agricultural productivity.
- b. The effect of the added acid was negligible.
- c. The impact of pesticide use on health is felt throughout the world.



“Whether” vs “Whether or not”

► Use “whether” to introduce at least two alternatives, either stated or implied.

- a. I am not sure whether I should repeat the experiment.
- b. I am not sure whether I should repeat the experiment or use a different statistical treatment.
- c. I am going to repeat the experiment whether the results are positive or negative.



► Use “whether or not” to mean “regardless of whether”.

Incorrect

- I am not sure whether or not to repeat the experiment.

Correct

- I am not sure whether to repeat the experiment.
- Whether or not the results are positive, I will repeat the experiment.
- Whether or not I repeat the experiment, I will probably leave the laboratory late tonight.



“to comprise,” “to compose,” “is composed of”

“to comprise” = “to contain” or “to consist of”

“to compose” = “to make up” or “to make”

The whole *comprises* the parts, or the whole *is composed of* the parts, but the whole is not comprised of the parts.

The parts *compose* the whole.

Never use “~~is comprised of~~”.



Incorrect

A book is comprised of chapters.

Correct

A book comprises chapters.

A book is composed of chapters.

Incorrect

Our research was comprised of three stages.

Correct

Our research comprised three stages.



The water molecule comprises two atoms of hydrogen and one atom of oxygen. ✓
(The whole comprises the smaller parts.)

The water molecule comprises of two atoms of hydrogen and one atom of oxygen. X
(Do not use the word *of* with *comprise*.)

Two atoms of hydrogen and one atom of oxygen comprise the water molecule. X



- Mercury, Venus, Earth and Mars compose the inner planets. ✓
- Two atoms of hydrogen and one atom of oxygen compose the water molecule. ✓
- USA is composed of 50 states. ✓
- The water molecule is composed of two atoms of hydrogen and one atom of oxygen. ✓



Use of “A” and “An”

► Choose the articles “a” and “an” according to the pronunciation of the words or abbreviations they precede.

a nuclear magnetic resonance spectrometer
an NMR spectrometer



► Use “a” before an aspirated “h”; use “an” before the vowel sounds of a, e, i, o, “soft” or “short” u, and y.

a house, a history (*but* an hour, an honor) a union,
a U-¹⁴C (*but* an ultimate)
a yard (*but* an ylide, an yttrium compound)

► Choose the proper article to precede B.A., B.S., M.A., M.S., and Ph.D., according to pronunciation of the first letter.

a B.S. degree; an M.S. degree; a Ph.D.



► Even when symbols are used, the element's name is pronounced. Therefore, choose the article (a or an) preceding the element symbol to accommodate the pronunciation of the element name.

- a. a Au electrode (pronounced "a gold electrode")
- b. a N-containing compound (pronounced "a nitrogen-containing compound")
- c. a He-Ne laser (pronounced "a helium-neon laser")
- d. a Ag/AgCl reference electrode



► The isotope name or symbol is pronounced first, then the number. Thus, ^{14}C is pronounced "c fourteen". Consequently, choose the article (a or an) preceding the isotope to accommodate the pronunciation of the element name or symbol, not the number.

- a ^{14}C isotope (pronounced "c fourteen")
- an ^3H isotope (pronounced "aitch three")
- an ^{15}N isotope (pronounced "en fifteen")



"That" vs "Which"

- 1 "That" is the right choice for restrictive clauses

Example

An approach **that** is based on perturbation theory offers...

- 2 "Which" is the right choice for nonrestrictive clauses

Example

This approach, **which** is based on perturbation theory, offers...

- 3 Consider a third option: no "which" or "that" at all:

Example

- "An approach based on perturbation theory offers..."
- "This approach, based on perturbation theory, offers..."



► Restrictive clauses are best introduced by “that”, not “which”.

- a. It was necessary to find a blocking group **that** would react with the amino group but not with the hydroxyl group.
- b. Comparison will be restricted to acetylene compounds **that** have the same functional end groups.

► If the clauses beginning with “that” were deleted, the sentences would not convey the information intended.



► Phrases can also be restrictive.

Reactions **leading to the desired products** are shown in Scheme 1.

► Nonrestrictive phrases and clauses are set off by commas. Nonrestrictive clauses may be introduced by “who” or “which” but not by “that”.

Squalene, a precursor of cholesterol, is a 30-carbon isoprenoid.



- a. This highly readable book, **written in nontechnical language**, surveys the field of chemistry by describing the contributions of chemistry to everyday life.
- b. Moore, **working at the Rockefeller Institute**, developed methods for the quantitative determination of amino acids.
- c. The current–voltage curves, **which are shown in Figure 6**, clearly demonstrate the reversibility of all four processes.



- a. Several hazardous waste disposal sites are located along the shores of the Niagara River, **which is a major water source.**
- b. Melvin Calvin, **who won the Nobel Prize in 1961,** elucidated the biochemical pathways in photosynthesis.
- c. James Aberdeen, **professor emeritus of Central State University,** **which has provided significant scholarship support to minority students over the years,** made a generous contribution to the school's building fund.



- a. The vial that contained her DNA was lost.
- b. The vial, which contained her DNA, was lost.
- c. Other disorders ~~which~~ **(that)** been found to co-occur with diabetes include heart disease and foot problems.
- d. When we say we are a pile of atoms, we do not mean we are *merely* a pile of atoms because a pile of atoms ~~which~~ **(that)** is not repeated from one to the other might well have the possibilities ~~which~~ **(that)** you see before you in the mirror.



“Where” vs “In which”

Where

This word is correctly used to refer to a place or a region (or to an equation...)

However, it should not be used for non-localised abstraction

Change:

a case where	to	a case in which
a situation where	to	a situation in which
a form where	to	a form in which

Change: “in the case in which” simply to “when”



“data” vs “datum”

► Data can be a singular or plural noun. In most cases, however, data is regarded as a plural, and its singular format is datum (rarely used).

Wrong:

The data suggests that...

Correct:

The data suggest that ...



Who vs. Whom

- Who does something (it's the subject, like he), and whom has something done to it (it's an object, like him).
- Try substituting he or him where who or whom should go: if he fits, you want *who*.
- Who** is it?
- She called to Beth, **who** (she believed) was nearby.
- [To] **whom** did you mean to call?
- The message was meant for **whom**?

As vs. like

Use “as” to introduce clauses (compare action)

We spent the evening as (we did) in the old days.

We wrote down every step, as good scientists should.

Use “like” (sparingly—more formal to use “similar to”) to compare nouns and pronouns

OK: Her cat is like a dog.

More formal: Her cat is similar to a dog.

BUT...

Her cat acts as a dog would.

Note: “Her cat acts similar to a dog” does not work.

Therefore, don't use ‘like’!



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Therefore, don’t use ‘like’!



Spectra vs. Spectrum

The word *spectra* is the plural form of *spectrum*. Use spectra with plural verb forms and spectrum with singular verb forms:

- The photoelectron **spectrum** **is** shown on the y axis.
- The NMR **spectrum** in the ring proton region **confirms** this assignment.
- The electronic absorption **spectra** of 4 and 5 **were** found to shift slightly upon addition of a metal ion.



Further vs. Father

Further (adjective/adverb/verb) indicates additional/additionally/to help or more/a great degree/to advance

- Further* proof is given by the observation of two titrating groups of equal contributions in the heme redox titration curve.
- The pH was immediately adjusted to 8.7, and the refolding mixture was *further* incubated with slow stirring at room temperature for 4 h.
- To further* our fundamental understanding of the underlying science, . . .



Farther (adjective/adverb) means more distant or at or to a great distance or more distant

- In the third case, the upper surface was moved a *farther* 0.74 Å to the right.
- When the concentration is higher, the metal ions move *farther* toward the maximum field.
- The magnitude becomes smaller because the chromophore is *farther* apart from the rim of the cavity of the chiral macrocyclic host.



Precede vs. Proceed

Precede (verb): to come, to occur before in time, order, rank, position, or place.

Preceding (a.j.): previous

Proceed (verb): to go forward, to begin an action or a process.

- The oxidative addition is *preceded* by decoordination of the anion.
- As mentioned in the *preceding* section, the reaction of . . .
- The thermal decomposition of 2,1-benzisoxazole will *proceed* at the lower temperature.



Writing effective paragraphs

- **Definition**
 - A series of sentences developing **ONE** topic
- **Three concepts for good paragraphs**
 - **Unity**: one idea per paragraph
 - **Development**: sufficient detail (good writing is 25% ideas & 75% details!)
 - **Coherence**: understandable, easy to follow (logical order, effective transitions)



Structure of a paragraph

- **Topic sentence**
 - Usually first—the topic of a paragraph is stated in **ONE** sentence.
- **Body**
 - The details which make your topic sentence vivid to the reader by developing or explaining the main idea.
- **Concluding sentence**
 - The last sentence of the paragraph. Restates the main idea. May prepare the reader for the following paragraph.



Example

Through the centuries rats have managed to survive all our efforts to destroy them. We have poisoned them and trapped them. We have fumigated, flooded, and burned them. Some rats even survived atomic bomb tests conducted in the Pacific after World War II. In spite of all our efforts, these enemies of ours continue to prove that they are the most indestructible of pests.



Linking words

- First
- Furthermore
- Another
- In addition to
- However
- On the other hand
- Consequently

Scientific Writing

V. Schemes, Figures, and Tables
(ChemDraw and OriginLab)

Dr. Wujian Miao



Graphics

Graphics: figures, tables, and schemes.

- Figures and tables are used to display, clarify, and summarize results, helping readers comprehend data more quickly.
- Schemes are used to illustrate mechanisms, reaction pathways, experimental setup, and working principles of proposed techniques...



Tables and figures

- Tables are appropriate for large or complicated data sets that would be difficult to explain clearly in text.
- Figures are appropriate for data sets that exhibit trends, patterns, or relationships that are best conveyed visually.
- Any table or figure must be sufficiently described by its title and caption or legend, to be understandable without reading the main text of the results section.
- Do not include both a table and a figure showing the same information



Attribute	Description
Repeated values	not included, state in table title/footnote (e.g., The temperature was 25 °C).
Size and orientation	Try to fit in one page. may exchange rows and columns, or break a long table into smaller ones. Avoid horizontal tables.
Spacing and empty cells	Single-space table titles and table entries to minimize unused space. No/few empty cells
Titles	Above table starting with an identifier (Table x.) and a brief, informative descriptor [either in sentence case (ending with “.”) or in title case], either left-justified or centered per journal requirements. e.g., Table 1. Reaction conditions for acid synthesis. Table 1. Reaction Conditions for Acid Synthesis



Electron Transfer in FeCl₂/OH in DMSO–Water *J. Phys. Chem. B, Vol. 106, No. 6, 2002 1393*

TABLE 1: Kinetic Parameters Obtained for the Oxidation of 1.00 mM FeCl₂/OH in Different Molar Fractions of DMSO Aqueous Solutions Containing 50.0 mM TMAP at a 5.06- μ m-diameter Pt Electrode ($T = 293$ K, except for t_{r} Values for 298 K)

χ_{DMSO}	ν^{a} (eP) ($\pm 0.55\%$)	D ($\times 10^6$) $\text{cm}^2 \text{ s}^{-1}$, $\pm 3\%$	D^{b} (L)	L	m_{e} ($\times 10^6$, $\text{cm}^3 \text{ s}^{-1}$)	k^{c} ($\text{cm}^3 \text{ s}^{-1} \pm 15\%$)	E^{d} (mV vs Pt) ± 3 mV	α (± 0.02)	t_{r}^{e} (μs)
0	1.602 ^f	7.8	2.95	0.204	15.51	2.66	48	0.20	0.44 ^f
0.10	2.152	3.7	4.00	0.200	7.452	1.93	50	0.19	0.38
0.20	3.455	2.5	3.99	0.201	5.022	0.43	70	0.32	2.16
0.30	4.31	2.0	4.06	0.197	4.088	0.20	75	0.31	3.94
0.33	4.383	1.9	4.02	0.199	3.845	0.14	71	0.36	4.47
0.37	4.354 ^g	2.0							
0.40	4.267	2.2	3.93	0.205	4.353	0.17	79	0.40	4.66
0.50	3.838	2.5	4.04	0.198	5.085	0.19	80	0.40	4.35
0.60	3.398	2.7	4.03	0.199	5.479	0.34	86	0.34	2.44
0.70	2.967	2.9	3.99	0.201	5.826	0.28	81	0.32	1.10
0.80	2.627	3.1	4.05	0.198	6.320	0.19	91	0.33	0.83
0.90	2.470 ^h	3.4	4.03	0.200	6.866	0.17	94	0.35	0.66
1.00	2.47 ^h	3.7	3.94	0.204	7.340	0.17	160	0.36	0.50

^a Viscosity from ref 25 unless otherwise stated. ^b From ref 16. ^c Interpolated values. ^d From ref 35. ^e Longitudinal relaxation time taken or interpolated from ref 21 unless otherwise stated. ^f Longitudinal relaxation time from ref 15.

Miao, W.; Ding, Z.; Bard, A. J. *J. Phys. Chem. B* **2002**, *106*, 1392-1398.



Schemes

- are used to depict a series of steps that **progress in time**.
- differ from charts, which list groups of compounds or structures that do not change in time.
- Most commonly, schemes are used to illustrate chemical reactions.
- often include arrows (e.g., to denote a forward reaction, resonance, equilibrium, and/or electron movement), intermediates, transition states, reactants, and products.



Demonstration and Practice with ChemDraw and OriginLab Software

The image displays two software interfaces. On the left is ChemDraw Pro 14 Suite, showing a chemical structure editor with a complex organic molecule (a substituted benzene ring with multiple hydroxyl and methyl groups) and a list of atoms on the left. On the right is ORIGIN 2016 Graphing & Analysis, showing a dashboard with several 3D surface plots and a 2D line graph. A small icon of a building is visible in the bottom right corner of the software window.

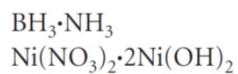
Scientific Writing

VI. Conventions in Chemistry

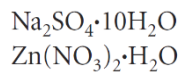
Dr. Wujian Miao



► In the formula for an *addition compound*, use a centered dot, closed up on each side.



Water of hydration follows a centered dot, closed up on each side.

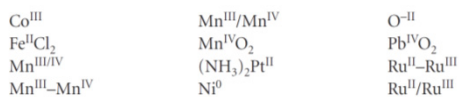


Use the Right Asterisk for Excited Electronic State



Use the Right Superscript for Oxidation Number

► You may use superscript roman numerals for oxidation numbers. In formulas, do not use numbers on the line to avoid confusion with the symbols for iodine or vanadium.



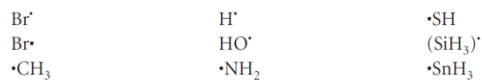
OR

cobalt(III) or Co(III)
copper(II) or Cu(II)

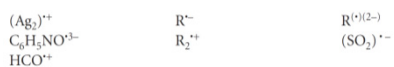


Radicals

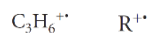
► free radicals



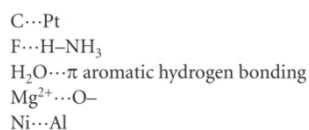
► Charged radical cations and anions



EXCEPTION: in mass spectrometry



► Use three centered dots to indicate association of an unspecified type (e.g., hydrogen bonding, bond formation, or bond breaking).



Abbreviations, Acronyms, and Compound Labels

Rule 1: To define an abbreviation or acronym, use the full term first, followed by the abbreviated form in parentheses [e.g., **electrogenenerated chemiluminescence (ECL)**]

Rule 2: Do not define abbreviations for elements (e.g., Fe), empirical formulas (e.g., **CH₃CH₃**), units (e.g., **mL**, **g**, **μm**, **°C**), or a few other commonly used chemical abbreviations (e.g., **DNA**, **NMR**).

Rule 3: Do not use an abbreviated term before it has been defined (unless it is a term that does not require definition).



Rule 4: Define an abbreviated term only once in the body of the work. After it has been defined, you may use it in the remainder of the work.

Rule 5: After an abbreviated term has been defined, you may still use the unabbreviated form if it seems more appropriate.

Rule 6: Avoid abbreviations and acronyms in titles.

Rule 7: If you define an abbreviation or acronym in an abstract or Project Summary, define it again in the body of the work.



Rule 8: Preface abbreviations and acronyms, when appropriate, with articles “a” and “an” according to the pronunciation (not the letter) of the first sound of the abbreviation or acronym: *a nuclear magnetic resonance spectrum, an NMR spectrum*.

Rule 9: Abbreviate units of measure when they follow a number. Without a number, spell them out:

e.g., 9 V/s measured in volts per second

Rule 10: Form the plural of multiple-letter, all-capital abbreviations and abbreviations ending in a capital letter by adding a lowercase “s” only. Do not put an apostrophe before the “s”; do not add an “s” to units of measure: PCBs, pHs, PAHs, CFCs, 10 mL



Rule 11: Use bolded numbers (e.g., **1, 2, 3, . . .**) and/or numbers and letters (e.g., **5a, 5b, 5c, . . .**) to represent chemical compounds.



Numbers and Units

Rule 1: Abbreviate units of measure (e.g., mL, cm, g, K), including units of time (e.g., s, h, min), when they follow a numeral. Do not use a period with an abbreviated unit (unless you are using the abbreviation for “inch”: in.).

Inappropriate	5 seconds	16 milliliters	13.5 in
Appropriate	5 s	16 mL	13.5 in.

Rule 2: Spell out units of measure if they do not follow a numeral.

Inappropriate	several mg a few min
Appropriate	several milligrams a few minutes

Rule 3: Use the numerical form of numbers (e.g., 7) rather than the word form (e.g., seven) with units of measure and time, unless the number is at the beginning of a sentence. Make sure you leave a space between the number and unit, unless you are using the % sign.

Inappropriate	seven mL/five cm/thirty percent/11 hours
Appropriate	7 mL 5 cm 30% 11 h

Rule 4: Use °C with a space after the number, but no space between the degree symbol and the capital C. For K (kelvin), include a space between the number and the K; do not use the degree symbol with kelvin.

Inappropriate	10°C 10 °C 10K 10 °K
Appropriate	10 °C 10 K

Rule 5: Do not add a plural “s” to make an abbreviated unit plural (unless you are using the plural form of spelled-out units, e.g., milligrams).

Inappropriate	4 mgs	4 mols
Appropriate	4 mg	4 mol

Rule 6: Use the word form of numbers less than 10, except when referring to units of measure.

Inappropriate	4 sites	five mg	thirteen sites	8 samples
Appropriate	four sites	5 mg	13 sites	eight samples

Rule 7: Do not define abbreviated units of measure (unless you are writing for a nonexpert audience).

Inappropriate	3 min (minutes)	300 mL (milliliters)
Appropriate	3 min	300 mL

Rule 8: Use numerals (not the word form) in a series or range containing numbers 10 or greater to maintain parallelism.

Inappropriate one, five, 10, and 15 mg, respectively
Appropriate 1, 5, 10, and 15 mg, respectively

Rule 9: In a series or range with a span of three or more numerals, include the unit of measure only once. Use the en dash to mean “to” or “through.”

Inappropriate 3 mL–10 mL 1 kg–4 kg
Appropriate 3–10 mL 1–4 kg



Exception 1 to Rule 9: When one or both of the numbers are negative or include a symbol that modifies the number, use the words “to” or “through” rather than the en dash.

Inappropriate –3–10 °C <2–4 kg
Appropriate –3 to 10 °C <2 to 4 kg

Exception 2 to Rule 9: Do not use the en dash when the words “from” or “between” are used.

Inappropriate from 200–400 mL between 1–3 h
Appropriate from 200 to 400 mL between 1 and 3 h



Rule 10: Use a slash (/), not the word “per,” for units of concentration when both units are abbreviated.

Inappropriate 20 µg per mL
Appropriate 20 µg/mL