Writing in Chemistry

HANDBOOK

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Handbook for Writing in Chemistry

Learning Objectives for Writing in the Major

Successful completion of the major coursework in chemistry or biochemistry means that students should be able to:

- identify and highlight salient information in experimental data through the use of properly formatted text, figures and tables.
- identify the library of primary sources in chemical literature, find and summarize relevant information and appropriately frame experimental results in the context of the primary literature.
- apply the most effective broad and fine organizational structures for research reports, grant proposals, and oral and poster presentations.
- create a credible scientific ethos though the use of appropriate grammar, mechanics, and conventions for professional scientific writing, especially the use of quantitative, accurate, and precise descriptions.
- keep clear and accurate records of experimental data that meet appropriate academic, industrial, and legal conventions for laboratory notebooks.
- identify strong and weak examples of these proficiencies in the work of others, especially peers, and propose ways to improve the effectiveness of these examples.

Important Writing Resources

The following two books will help you significantly as you develop as a writer. Both of these books can be found in the Murphy Library, however if you intend to pursue chemistry as a career, it is worth your money to buy copies of both.

- Coghill, A. M.; Garson, L. R. *ACS Style Guide: Effective Communication of Scientific Information;* an American Chemical Society Publication, 2006.
  This is the official style guide for the American Chemical Society and the official source for answers to questions regarding style and formatting.
- Robinson, M. S.; Stoller, F. *Write like a chemist: a guide and resource;* Oxford University Press US, 2008.
  This book is the result of an NSF-funded project to improve writing instruction in chemistry and is indispensable if you are interested in learning how to write chemical writing genres. It presents a structured approach to writing research reports, posters, grant proposals and conference abstracts and contains some of the most detailed and insightful information on chemistry writing available.

Accuracy, Precision, and Concision

“Concision in style, precision in thought, decision in life.” -V. Hugo

The purpose of scientific communication is to communicate effectively and efficiently. Therefore, scientific writing must be accurate, precise, and concise. The following guidelines will help you improve your ability to write according to these standards.

Accuracy
Accuracy in scientific writing means that all statements are correct, not simply the main idea. Lack of complete understanding of a topic is the most common source of inaccurate writing. To prevent this, be sure to review your writing to make sure you understand every statement you include and that it is correct. If you do not understand something, consult your instructor or course materials.

Precision
Precise writing means that the identity of every noun and pronoun is clear and that the subject of every verb is clear. Lack of precision is most often the result of ambiguous pronouns (it, they, etc.) but can also result from a lack of definition between two or more possible identities for a word (e.g. "the reagent," when more than one reagent is present). Be sure to review your writing to make sure that the subject of each noun, pronoun and verb is well defined.

Examples

Accurate and Precise

- The acid reacts with the sodium bicarbonate to create carbonic acid, which breaks down on its own to make carbon dioxide.
- Acid reacts with bicarbonate to create carbonic acid, which breaks down into water and carbon dioxide.

Accurate But Not Precise

- It's breaking down because it's being reacted with the acid.
- Because it is giving off carbon dioxide.

Precise But Not Accurate

- The diatomic hydrogen gas created from the reaction of the acid and the bicarbonate.
- The bubbles that form are made up of carbon dioxide gas that formed when the water reacted with carbon.

Neither Accurate Nor Precise

- The sodium bicarbonate is a base that interacts, making it bubble.
- There is a chemical reaction occurring to neutralize it.

Concision
"Vigorous writing is concise. A sentence should contain no unnecessary words, a paragraph no unnecessary sentences, for the same reason that a drawing should have no unnecessary lines and a machine no unnecessary parts." -W. Strunk

Concise writing shows that you know which information is most important to your reader. However, no writing begins concise, concision is always the product of multiple rounds of revision. Thus, you will need to plan for multiple revisions in order to determine which elements are most essential, and the most efficient way to state them. The following examples of revising writing for concision will help you approach editing your own writing.

Examples

*First, **identify and eliminate words that are redundant or provide no extra meaning.***

- Chromatography is an experimental technique used by chemists *as a means to help them* separate *different* compounds in experimental samples using the affinity of the compound for the mobile phase as well as the affinity of the compound for the stationary phase. [42 words]

- *A piece of* B&S no. 24 copper wire *that was 49.7 cm in length was massed and found to weigh* 0.85 g. *The sample* was rolled into a flat coil and placed in a 150 mL beaker. A *dilute* nitric acid solution *was prepared by pouring 10 mL of 8M nitric acid into 10 mL of water. The nitric acid solution* was added to the copper in the 150 mL beaker. Changes were noted. A hot plate was used to speed up the reaction. The reaction continued until all the copper had reacted. [93 words]

Next, ***remove information that you can assume your reader already knows*** *(this requires knowing your audience).*

- Chromatography is an experimental technique used by chemists to separate compounds *in experimental samples* using the affinity of the compound for the mobile phase as well as the affinity of the compound for the stationary phase. [36 words]
- A 0.85 g sample of B&S no. 24 copper was rolled into a flat coil and placed in a 150 mL beaker. 20 mL of 4.0 M nitric acid solution was added to the copper. Changes were noted. A hot plate was used *to speed up the reaction. The reaction continued* until all the copper had reacted. [57 words]

Finally, ***look for more concise ways of saying the same information.***

- Chromatography *is used to separate compounds using the affinity of the compound for the mobile phase as well as the affinity of the compound for the stationary phase.* [28 words]
- *A 0.85 g sample of B&S no. 24 copper was rolled into a flat coil and placed in a 150 mL beaker. 20 mL of a 4.0 M nitric acid solution as added to the copper. A hot plate was used until all copper was reacted.* [46 words]

Final Result

- Chromatography separates compounds based on the affinity of the compound for the mobile phase relative to the stationary phase. [19 words]
- 20 mL of 4.0 M nitric acid was added to 0.85 g of rolled B&S copper in a 150 mL beaker and heated until all of the copper was reacted. [30 words]

Describing and Interpreting Data

"The idea is to try to give all the information to help others to judge the value of your contribution; not just the information that leads to judgment in one particular direction or another." -R. Feynman

There is an important distinction between descriptions of experimental observations and the interpretation of their meaning. Effective discernment between a description and an interpretation of data is one of the hallmarks of a good scientist.

Description of Data

Descriptions of data include correlations, comparisons, maximum or minimum values, or anything else that can be directly observed from the data. Descriptions of observations are certain, and can be stated as simple facts.

Examples

- The titration reached the inflection point when 2 moles of sodium hydroxide were added to 1 mole of oxalic acid.
- A blue precipitate was formed when the unknown solution and sodium bicarbonate were combined.
- The excited hydrogen atoms emitted light at 410.2 nm.

Interpretation of Data
In contrast, interpretation of data involves using the laws and theories of science to infer what the data tell us about proposed hypotheses. Because interpretations are based on inference rather than direct observation, statements regarding interpretations are more qualified.

Examples
- This implies that oxalic acid is a diprotic acid.
- Therefore, the unknown solution appears to be copper nitrate.
- This is consistent with the prediction of the Schrödinger wave equation for hydrogen electrons falling from the n = 6 to n = 4 energy levels.

Formatting

Formal Figure Formatting Guidelines
"The commonality between science and art is in trying to see profoundly – to develop strategies of seeing and showing." -E.R. Tufte

Figures are the essential method of summarizing experimental results and form the foundation for almost all scientific reports. A good figure not only shows data, it highlights the meaning behind the data. Well-formatted figures illustrate experiential trends and key observations while minimizing visual distractions. The following guidelines will help you construct clear and concise scientific figures that minimize visual clutter.

Presentation of Data
- Independent values are plotted on the x-axis, dependent values on the y-axis.
- In general, no more than five curves to a figure. (May be more or less if scientifically necessary.)
- Identity of each curve is clear.
- Curves are spaced to maximize their visibility.
- Scaling is not deceptive, minimizes white space.

Text and Axes
- Fonts are same size as text. (Axis labels can be one font size larger.)
- Axes un-bolded, first letter capitalized, units in parentheses with standard abbreviations outside and parallel to axis.

Captions and Legends
- No title in figure.
- Captions are below figures, aligned to the left, with identifier in bold (in fragment form), contains additional information identifying figure independently from rest of text, same text size as rest of text.
- Each figure is numbered consecutively with Arabic numerals.
- Legends are integrated into the caption or put on the figure with no surrounding box in a place that does not obscure the data.

Use of Color
- Figure is in black and white (unless color enhances presentation of the science).
- Background is white, no grid lines on background (unless scientifically necessary).
- Black/white contrast between symbols is maximized and choice of symbols reflects organization of data. (Example: filled symbols with inhibitor, open symbols without.) Avoid close shades of gray.

Formal Table Formatting Guidelines

"The goal is to transform data into information, and information into insight." -C. Fiorina

When actual values are essential, or data cannot be summarized well in a figure, it is useful to use a table. However, tables are not simple lists of numbers. As with graphs, a well-constructed table highlights the most important trends and patterns in data and minimizes visual distractions. The following guidelines will help you construct clear and concise scientific tables.

Presentation of Data

- Columns ordered with independent variables on left, dependent variables on right reads from left to right in progress of values.
- Frequently repeated values are placed in footnotes or the table title instead of in table.

Text and Numbers

- Font is same size and type as rest of text, all fonts the same in table.
- Text is single spaced and left justified.
- Numbers aligned around decimal place.
- Lowercase (unless normally capitalized) letters used in column entries.

Titles, Headings, and Footnotes

- Title is above body of table, contains an identifier (usually not a complete sentence).
- Each table is numbered consecutively with Arabic numerals.
- All columns have headings.
- Column headings are un-bolded.
- Units after heading in parenthesis, or directly below heading.
- Footnotes used to indicate specific information, all footnotes reference in table using superscripted lowercase letters (a, b, c, etc.) placed beneath table in same font.

Size, Lines, and Color

- Table is in black and white.
- Table conforms to page and column size limitations.
- Table contains the minimum white space possible.
- Tables contains only horizontal lines. (Generally one at top and bottom of table and one below column headings.)

Citation and Reference Formatting Guidelines

"There are no answers, only cross references." -Anonymous

The easiest way to manage and cite references is to use citation management software such as Zotero or Endnote. These programs are a convenient way of storing your references in one place (most will link directly to .pdf files on your computer), and can automatically insert and format references for you using the appropriate style in a number of different word processing programs. However, it is important to understand the basic rules of formatting citations so that you can use these programs intelligently.

The following guidelines are for citing and formatting references in the general ACS style. Since variations exist across different ACS publications, be sure to check with your instructor to determine if these guidelines are appropriate for your assignments.

Citing References in Text

- Citations are located in a logical place in sentence.
- Superscript or italic numbers in parenthesis are used to mark citations (depending on discipline).
- Numerical references start with 1 and are numbered consecutively throughout the paper.
- Multiple numbers are separated by commas, and sequential numbers are hyphenated.
- If a reference is repeated; the original reference number is used.
- If a reference has two authors; both names are given joined by "and."
- If a reference has more than two authors; the first name followed by "et al." is used.
- If more than one reference by the same principle author with various coauthors are cited, the principle authors name followed by "and co-workers" is used.

Examples

Parenthesis – Rees et al. (5) observed that the destabilizing effect of GB on DNA increases with increasing fraction of GC basepairs.

Superscript – Rees et al.[5] observed that the destabilizing effect of GB on DNA increases with increasing fraction of GC basepairs.

Parenthesis – Results of these studies have been analyzed by Record and co-workers using the solute partitioning model. (1-4, 17, 18)

Superscript – Results of these studies have been analyzed by Record and co-workers using the solute partitioning model.[1-4, 17, 18]

Formatting Reference Lists

Examples of reference formatting using ACS style are found below. Specific details on the formatting of references can be found in the *ACS Style Guide.*

Article in a Scientific Journal – Evans, D. A.; Fitch, D. M.; Smith, T. E.; Cee, V. J. Application of Complex Aldol Reactions to the Total Synthesis of Phorboxazole B. *J. Am. Chem. Soc.* **2000**, 122, 10033-10046.

Article from an Online Journal – Peacock-Lopez, E. Exact Solutions of the Quantum Double Square-Well Potential. Chem. Ed. [Online] **2007**, 11, 383-393 http://chemeducator.org/bibs/0011006/11060380lb.htm (accessed Aug 23, 2007).

Article Published Online in Advance – Chung, J.M. and Peacock-Lopez, E. Cross-diffusion in the Templator model of chemical self-replication. Phys. Lett. A [Online early access]. DOI:10.1016/j.physleta.2007.04.114. Published Online: June 12, 2007. http://www.sciencedirect.com (accessed Aug 23, 2007).

Single Author Book – Chang, R. *General Chemistry: The Essential Concepts,* 3rd ed., McGraw-Hill: Boston, 2003.

Edited Book – Gbalint-Kurti, G. G. Wavepacket Theory of Photodissociation and Reactive Scattering. In *Advances in Chemical Physics;* Rice, S. A., Ed.; Wiley: New York, 2004; Vol. 128; p 257.

Book in Series – *Omega-3 Fatty Acids: Chemistry, Nutrition, and Health Effects;* Shahidi, F., Finley, J. W., Eds.; ACS Symposium Series 788; ACS: Washington, DC, 2001.

Article from a Reference Book – Powder Metallurgy. *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed.; Wiley: New York, 1982; Vol. 19, pp 28-62.

Computer Program – *SciFinder Scholar*, version 2007; Chemical Abstracts Service: Columbus, OH, 2007; RN 58-08-2 (accessed Aug 23, 2007).

Formatting for additional types of citations can be found in the *ACS Style Guide.*

Text Formatting Guidelines

"Information is a source of learning. But unless it is organized, processed, and available to the right people in a format for decision making, it is a burden, not a benefit." -W. Pollard

Chemical scientific writing should be formatted according to the conventions outlined in the *ACS Style Guide.* Not formatting your text to professional standards reduces legibility and reduces your professional credibility. Some key formatting guidelines for chemical research reports are outlined below. For a more detailed list of formatting information, consult the *ACS Style Guide.*

Abbreviations

You should define abbreviations upon first use, however certain abbreviations have been deemed common enough that they don't need to be defined. (See *ACS Style Guide.*) Here are some guidelines for using abbreviations:

- Use standard abbreviations whenever possible. (See *ACS Style Guide* for a list.)
- Use "e.g.," "i.e.," "vs." and "etc." in captions, tables and parenthesis. Elsewhere spell out "for example," "that is," versus," and "and so forth."
- Form the plurals of multi-letter all-capital abbreviations, and other abbreviations ending in a capital letter with a lowercase s only, no apostrophe.
- Add apostrophe to "s" of all lowercase abbreviations to form plural.
- Use Greek letters, not the corresponding spelled out words, for chemical and physical terms.
- When creating abbreviations they:
    - should not be identical to any unit of measure.
    - should not be able to be confused with any element or group.
    - should not hamper reader's understanding.
    - should not use same abbreviation for more than one spelled out form.

Capitalization

The *ACS Style Guide* gives detailed guidelines for which words should be capitalized in which contexts. Some of the more common situations are summarized below.

Capitalized

- "Figure," "table," "chart," or "scheme" when they refer to a specific numbered item.
- Genus names (when used as formal names).
- Main words: nouns, pronouns, verbs, adjectives, adverbs, subordinate conjunctions and English part of chemical descriptors in titles and headings.

Not Capitalized

- Abbreviated units in titles or heading if ordinarily lowercase.
- Surnames that are units of measure unless otherwise indicated. (See *ACS Style Guide.*)
- The locant, stereoisomer descriptor or positional prefix in a chemical name unless otherwise indicated. (See *ACS Style Guide.*)
- "As" in titles when used as preposition.

Hyphenation

Hyphens are used in a number of contexts in scientific technical writing. A few general guidelines are listed below. For a more detailed explanation and a list of the many exceptions to these guidelines, you should refer to the *ACS Style Guide.*

- Most prefixes are not hyphenated.
- Most suffixes are not hyphenated.
- Unit modifiers (two words that together describe a noun) are almost always hyphenated.

Typefaces
Choice of typeface (roman, italic, boldface, etc.) for text is also defined by ACS style guidelines. In general, roman type is used for most text, while italic typeface should be used for the following purposes:

- To emphasize words or phrases. (Use sparingly; do not use it for long passages.)
- Words being defined or when newly introduced terms appears in text for first time.
- Titles and abbreviation of periodicals, books and newspapers.
- Genus and species when used specifically.

Mathematical Expression Formatting Guidelines
"Pure mathematics is, in its way, the poetry of logical ideas." -A. Einstein

Some key formatting guidelines for the use of mathematical expressions in chemical research reports are outlined below. For more detailed formatting information, as well as many examples, consult the *ACS Style Guide.*

Numbers

- Use numbers before and after a decimal point (0.2, not .2 and 14.0, not 14).
- Use numerals for expressions used in a mathematical sense.
- For very large or small numbers with units of measure do one of the following:
    - Use scientific notation.
    - Choose an appropriate multiplying prefix to avoid numerals larger than four digits.
- Do not use e or E to mean "multiplied by the power of 10."
- With items other than units of time or measure, use words for cardinal numbers less than 10, use numerals for 10 an above.
- Spell out ordinals "first" through "ninth." Use numerals for 10th or greater.
- When a sentence starts with a specific quantity, spell out the number as well as the unit of measure. If possible, recast the sentence.

Mathematical Expressions

- Define all symbols for mathematical constants, variables and unknown quantities the first time they are used in the text.
- Do not use an asterisk to indicate multiplication.
- If an equation is very short and will not be referred to again, you may run it into the text.
- For equations that are not run into the text, number them by using any consistent system of sequencing. Place the identifier in parentheses, flush right on the same line as the equation.
- Following a displayed equation that is part of a sentence, punctuate the text as if it were a continuation of a sentence including the equation. (In most cases a colon is usually inappropriate for introducing a displayed equation because the equation finishes a phrase or sentence.)
- To cite an equation in text, use the abbreviations "eq." or "eqs." if it is not the first word of the sentence. Spell out "equation" when it is the first word of a sentence, or when it is not accompanied by a number.
- Spaces are included:
    - before and after (most) mathematical signs used as operators, except in superscripts and subscripts.
    - before trigonometric and other functions set in type.
    - after functions set in type when their arguments are not in enclosing marks.
    - between functions as components of products.

- Spaces are not included:
    - between single-item variables being multiplied.
    - in any part of a superscript or subscript, unless confusion or misreading would result.
    - between any character and its own superscript, prime, or subscript.
    - after mathematical operators used as an adjective (such as the > in >9).
    - between an opening parenthesis, bracket, or brace and the next character.
    - between a closing parenthesis, bracket, or brace and the previous character.

Formatting Units

- Where possible, use metric and SI units in all technical documents.
- Abbreviate units of measure when they accompany numerals. Do not use a period after an abbreviated unit of measure: exception: in. for inches.
- Use a space between the number and the unit: exception: %, $, angular degrees, minutes and seconds (°, ’, ’’).
- Write abbreviated compound units with a center dot or a space between the units to indicate multiplication and a slash or negative exponent for division. (Enclose compound units following a slash with parenthesis.)
- °C has no space between ° and C.
- Do not use the degree symbol with Kelvin.

Standard Deviation and Error

Standard deviation, standard error, or degree of accuracy can be given in two ways:

- With only the deviation of the least significant digits placed in parentheses closed up to and following the main numeral.
- Preceded by a ± following the main numeral, spaces are left on each side of the ±.

Chemical Names, Expressions and Reaction Formatting Guidelines

“I feel sorry for people who don’t understand anything about chemistry. They are missing an important source of happiness.” -L. Pauling

Formatting Chemical Names

Chemical compounds are named according to the rules established by the International Union of pure and Applied Chemistry (IUPAC), the International Union of Biochemistry and Molecular Biology (IUBMB), the Chemical Abstracts Service (CAS), the Committee on Nomenclature of the American Chemical Society, and other authorities as appropriate. For rules on naming compounds consult http://www.chem.qmul.ac.uk/iupac/. The following guidelines are for formatting names that are presumed to be correct.

Locants and Descriptors

Locants indicate the position of a functional group within a molecule. Descriptors indicate other properties (stereochemical, configurational, etc.) about functional groups. These are formatted as follows:

- Use commas between numeral locants, chemical element symbol locants, and Greek locants, with no space after the comma.
- Use hyphens to separate locants and configurational descriptors from each other and from the syllabic portion of the name.
- Use italic type for positional, stereochemical, configurational, and descriptive structural prefixes when they appear with the chemical name or formula.

- Use Greek letters, not the spelled out forms, in chemical names to denote position or stereochemistry. Use a hyphen to separate them from the chemical name.
- When structural prefixes are integral parts of chemical names, close them up to the rest of the name and do not italicize them.

Other Text

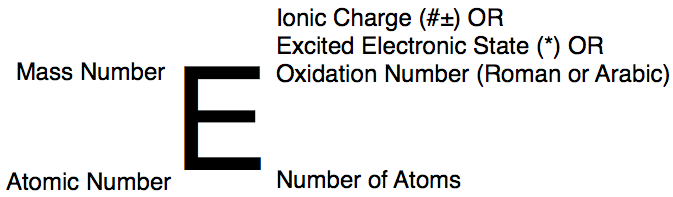
Treat the word or syllabic portions of chemical names just like other common nouns (roman, typically lowercase except at start of sentence or in titles or headings).

Amino Acids

- Always capitalize the three-letter and one-letter abbreviations for amino acids.
- Separate the three-letter abbreviations with hyphens.
- Do not use abbreviations for individual amino acids in running text.

Formatting Chemical Symbols

Superscripts and subscripts to an element follow the following conventions:



- Stagger subscripts and superscripts, place the subscript first.
- Mass number and atomic number are usually omitted unless relevant to topic of discussion.
- Oxidation numbers can also be written on the line in parenthesis closed up to the element name or symbol. (Example: copper(II).)
- Isotopes can be specified in text by spelled out name hyphenated to mass number. (Example: a carbon-14 isotope.)

Formatting Reaction Equations

- Short reactions may be run into text or displayed and numbered.
- Long reactions should be displayed separately from the text.
- Many different arrow symbols can be used. The following are some common examples:
  - ⇌ is used for a reaction proceeding in both directions.
  - ⇋ is used to indicate a reaction that is in equilibrium.
  - ⟷ indicates resonance structures, not a reaction.
- To indicate the aqueous, solid, liquid or gas state, use the appropriate abbreviation in parentheses, with no space preceding them.
- Indicate reaction conditions and catalysts over and under the arrow in a smaller type size:
  - Δ is used to denote heat.
  - hv is used to denote light.

Organizing Your Writing

"First comes thought; then organization of that thought, into ideas and plans; then transformation of those plans into reality. The beginning, as you will observe, is in your imagination." -N. Hill

Broad Organizational Structure

Scientific papers and posters are typically organized into four major sections: Introduction, Methods, Results and Discussion. These four sections constitute the broad organizational structure of a paper. The purpose of each of these sections is summarized as follows:

- Introduction – Introduce the research area and proposed work.
- Methods – Describe the materials and methods used in the study.
- Results – Summarize and highlight the most important observations and trends.
- Discussion – Interpret most important results and summarize general implications of work.

Fine Organizational Structure

Good research reports do more than just list relevant information, *they are organized to show the reader which pieces information are most important and how they relate to one another.* This level of organization is called the fine organizational structure of a report and is essential for good writing. The following outline will help you to select the most essential information needed in each section of a formal research report, and assist you in arranging it most effectively.

Introduction

1. Introduce the Research Area
   1.1. Identify the research area.
      a. *What theories are used in this study?*
      b. *What molecules are the subjects for this study?*
      c. *What experimental approach is used for this study?*
      d. *Of these, which topic does the paper aim to provide the most significant new knowledge about? (This is the research area of the paper.)*
   1.2. Establish the importance of the research area.
      a. *Why would learning more about this research area be beneficial?*
   1.3. Provide essential background information.
      a. *What does the reader need to know about:*
         i. *the theories used in this study?*
         ii. *the molecules used in this study?*
         iii. *the experimental methods used in this study?*
2. Identify a Gap
   What information about the research area still needs finding out?
3. Fill the Gap
   3.1. Introduce the current work.
      a. *What is the goal of this study?*
      b. *How will it be accomplished?*
      c. *Summarize the final results and conclusions of the study.*

Materials and Methods

1. Describe Materials
   a. *List all the materials used in this study. Include source and purity.*
2. Describe Experimental Methods
   a. *List the experimental methods used in this study.*
   b. *List the major steps in each method.*
   c. *List the instruments used. Include manufacturer and model number.*
   d. *List any essential software used.*
   e. *List the equations used for any calculations used to convert raw data to final results for each method.*
3. Describe Numerical Methods (if present)
   a. *List any computational methods used separately from initial analysis of experimental results.*

Results

1. Set the Stage
    1.1. Remind reader how results were obtained.
        a. *Make a list of figures/tables that summarize results of the study.*
        b. *Summarize what experiments were done to obtain each figure or table?*
    1.2. Refer readers to a graphic that displays results.
        a. *List your observations about each figure or table. Mark the one to three most important observations for each figure or table.*
        b. *What trends do you see in each figure or table?*
        c. *Is there anything unexpected in any figure or table?*

Discussion

1. Discuss Specific Results
    1.1. Remind reader of results.
        a. *List the major results identified in the previous section.*
    1.2. Interpret results.
        a. *Interpret what each result means about the goals of this study.*
2. Conclude the Paper
    2.1. Summarize the work.
        a. *Summarize the goals, methods and results of this study*
    2.2. Suggest overall implications/applications of work.
        a. *State the new information contributed to the research area of this study.*

More information about broad and fine organization in scientific papers, posters, and grant proposals can be found in the book *Write Like a Chemist,* which also summarizes the major fine organizational structures in scientific writing in Appendix A.

Correct Use of Grammar, Tense, and Voice

"Grammar is the logic of speech, even as logic is the grammar of reason." -R. C. Trench

Grammar and Mechanics Guidelines

You are expected to use correct English grammar in all of your written work. While a review of basic grammar is outside the scope of this handbook, the following are some of the more common grammar and mechanics issues to watch for in scientific writing.

- All words should be spelled correctly.
- Commas, periods, colons, quotation marks, parentheses, dashes, brackets and semicolons must be used appropriately.
- Subjects and verbs should all agree in number.
- No necessary verbs are omitted from the text.
- Restrictive (necessary to meaning of the sentence) and nonrestrictive (adds information but not essential) expressions are used correctly.
- No dangling modifiers (a word or phrase that does not clearly and logically modify another word in a sentence) are present.

See the *ACS Style Guide* or a grammar reference book (for a good read, choose *The Deluxe Transitive Vampire* by Karen Gordon) for more details on and examples of each of these grammatical rules.

Tense and Voice

Certain conventions for the use of both tense and voice exist in scientific writing. In general, "eternal" truths are referred to in the present tense, while specific events are referred to in the past tense. The following table summarizes some of the appropriate verb tenses and voices to use in the four sections of a formal research report. For expanded lists and examples, refer to Tables 3.4, 4.1, 5.1, and 6.5 in *Write Like a Chemist.*

Selected Conventional Uses of Tense and Voice in Scientific Writing

Section	Purpose	Tense/voice
Introduction	-To introduce research area -To provide relevant background information -To identify a gap -To introduce current work -To hint at findings in past work	-Present-active -Present-active -Present-active -Present-active -Past-active or passive or Present-active
Methods	-Anything	-Past-passive
Results	-To describe specific results -To state scientific "truths" or knowledge -To refer to a figure or table	-Past-active -Present-active -Present-active or passive
Discussion	-To remind readers what was studied in current work -To interpret results presented in the current work -To propose "truths" based on the current work and other's works -To suggest overall implications and/or applications of the current work	-Past-active or passive -Present-active -Present-active -Present-active

Writing About Primary Chemical Literature

"I have gathered a posie of other men's flowers, and nothing but the thread that binds them is mine own."
- John Bartlett

- In scientific writing, primary literature is cited to provide background information and to support conclusions. When you write about research results found in the primary literature you will want to keep in mind the following points.
- When summarizing background literature, keep to the most important references rather than summarizing all available literature. This provides focus and improves concision.
- When citing references from the literature, be concise. (Follow the pattern illustrated in this handbook for editing your citations.)
- Do not use direct quotations of articles. Scientific writing values concision more than reproduction of the original wording. Instead, summarize the essential information (methods, specific results or general conclusions) you want the reader to know about the report.

Examples

A change of the vibrational density of states, g(ω), on binding MTX to DHFR at 120 K has been observed using inelastic neutron scattering.[17]

Lee and Richards pioneered the calculation of water-accessible surface area (ASA) of proteins and model compounds and initiated the use of ASA in analyses of protein stability. (21)

- To make your writing more concise, summarize multiple similar studies into a single summary statement.

Examples

The transition state structure of human PNP has permitted the design of several transition state analogues with picomolar dissociation constants. (3-7)

In the absence of DNA, the structure of the bHLH domains studied to date is disordered. (16-18)

Notebook Construction

"Remembering the past gives power to the present." -Anonymous

A laboratory notebook is an important part of experimental research. Without a permanent record of your experimental methods and results it is nearly impossible to write research reports or design new experiments. Therefore, it is important to organize your lab notebook so that you and others can quickly find and understand the information it contains. The following guidelines will help you produce a clear and permanent record.

Notebook Guidelines

- Each page is dated.
- Permanent materials (ink, hard bound, etc.) are used.
- All data is represented in its original form (taped in copies of computer printouts, original number of decimal places from readings, etc.) and clearly labeled.
- All procedures followed are outlined in sufficient detail that experiment can be reproduced by others (instrument settings, concentrations, volumes, masses, etc.).
  - *Weak:* Measured absorbance.
  - *Strong:* Measured absorbance of standard samples at 595 nm in a Spec-20 spectrophotometer.
  - *Weak:* Added inhibitor.
  - *Strong:* Added 0.5 mL of 10 mM NaH_2PO_4.
- Detailed description of the purpose of session is indicated at start of recording session.
  - *Weak:* Using a standard curve.
  - *Strong:* Determine the concentration of an unknown $KMnO_4$ solution based on the absorbance of standard $KMnO_4$ solutions.
  - *Weak:* Purify fumarase.
  - *Strong:* Use Ni-NTA chromatography to purify recombinant His-tagged fumarase from E. *coli* cells.
- Most significant conclusions are summarized in detail at end of experiment.
  - *Weak:* Purification was successful.
  - *Strong:* Changing protease inhibitors increased final purity 5-fold and resulted in a 95% yield.
  - *Weak:* Concentration of solution successfully found.
  - *Strong:* The concentration of the unknown solution was determined to be 0.45 ± 0.2 mM.

Writing Peer Reviews

"Lead yourself, lead your superiors, lead your peers, and free your people to do the same. All else is trivia."
-D. Hock

The following questions can help you come up with useful and insightful comments about how to improve both your own on other's writing. Review the relevant sections of this handbook for more information on each topic.

Reviewing Editing and Style

- Are the following formatted correctly?
    - *Figures and tables*
    - *Citations and references*
    - *Text, numbers, and mathematical or chemical expressions*
- Are grammatical rules applied correctly?
- Are the appropriate tenses and voices used in each section?

The Editing and Style checklists in Appendix A can assist you in evaluating formatting, grammar and style issues.

Reviewing Scientific Content

- Is the information organized into the appropriate structures for chemical writing genres on both a broad and fine level?
- Does the writer distinguish between description of experimentally observable evidence and interpretation of that evidence in terms of scientific models and theories?
- How successful is the reader at synthesizing multiple elements of content knowledge, including information from the primary chemical literature into a single picture?
- Is the language accurate and precise?
- Can the writing be made more concise?

The grading criteria tables in Appendix B can assist you in evaluating these skills.

Appendix A **Checklists for Writing Mechanics and Style**
Appendix B **Grading Criteria for Scientific Critical Thinking Skills**