Writing Style and Manuscript Organization
Adapted from "Writing a Scientific Manuscript: Highlights for Success", T. Spector (1994) J. Chem. Ed, 71, 47-50 and “Guidelines for Writing Scientific Journal Articles” from the University of the Ozarks, Biology Department (Division of Experimental Therapy, Burroughs Welicome Co., Research Triangle Park, NC 27709)

Many scientists are far more comfortable performing scientific experiments than they are reporting their findings. Although they could benefit from the excellent resources available on scientific writing, they may not have time to read these comprehensive articles. As a result, considerable data either are not reported or are published in ways that inadequately express their significance.

This article was written to complement the extensive reviews. It presents techniques for optimally relaying the content and meaning of scientific studies and for avoiding common problems. It begins with key features of the standard journal sections, tables, and figures and suggests strategies for their effective construction. It then discusses simple strategies to construct succinct sentences that are easy to read and understand.

Side Note: You are required to download a full article (on a synthetic organic chemistry topic) from the Journal of the American Chemical Society (JACS; can be accessed online through LIAS) before writing your final report. Your final report should be double-spaced and follow the JACS format as described below (under Manuscript Sections).

Manuscript Sections

Titles

Although the details of the title page are specified in the instructions for each journal, suggestions for title selection may not be adequate. Titles should be short, revealing, and enticing, but generally do not contain an active verb. Because most people scan titles by looking at their beginning and ending, the most important words should be located in these places. A bold phrase or name (heading) ending with a colon and followed with a descriptive phrase (subtitle) provides initial recognition plus crucial information.

Title Example:
“Facile Preparation of Tetra(2-aminoethyl)methane and Tetra(3-aminopropyl)methane: Novel Tetravalent Monomers for Materials Synthesis”

Author Line

This part of the paper is where your name and the names of collaborators/co-workers; usually done in order of the author who did the most work or, if work was equal, then in alphabetical order. The principle investigator’s name (usually the research professor) is followed by an asterisk; this name may appear first or last. It also includes the place(s) where the work was done.

Example:
Ken S. Feldman* and Katherine M. Masters
Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania 16802

Summary/Abstract

An abstract summarizes your paper or presentation in one concise paragraph (usually less than 250 words). The abstract should state the object of the project, methods employed, summarized results and primary conclusions. It is usually easiest to write the abstract after completing the other sections of the paper. An example follows.
Abstract Example:
A model 1-naphthoic acid bearing a peri-positioned cinnamic acid residue crystallizes as a closed H-bonded dimer. Irradiation of this crystalline solid provides \(\alpha\)-truxillate-type cyclobutane photodimer in quantitative yield. Further synthesis studies have led to more highly functionalized naphthoic/cinnamic acid species capable of (pseudo)centrosymmetric attachment to polyvalent hubs. This system demonstrates the feasibility of designing a covalent molecular connector whose orientation is encoded by its H-bonding pattern.

Introduction

This is the most important section for manuscript construction. It provides background information that describes and justifies the need for or advantage of the scientific study. It then clearly defines the purpose or problem, explains the approach taken, and may end with a brief summary of the findings. Thus, a well-written introduction structures the entire manuscript. Authors who write this section first usually find that the rest of the manuscript readily flows from it.

Introduction Necessities:
1) Why did the author undertake this study? The best initial statement is often a description of an observation in nature, or a conclusion drawn from a survey of the literature, that stimulated the interest of the author.

2) What is the existing state of knowledge of this topic? The author should synthesize information from the literature into an account that traces the development of the problem and summarizes its current state. In particular, gaps or inadequacies of current knowledge should be identified.

3) What is the author going to do? He or she must indicate specific objectives or hypotheses that will be tested. These should be clearly spelled out and in the case of hypotheses, should be statements that are capable of being either supported or refuted by the planned work.

Results

This is usually the most straightforward and easiest section to write. Results should contain an objective and clear description of the experimental findings presented in a logical sequence that unravels the story and aids the reader's understanding. This sequence is not necessarily the chronological order in which the experiments were performed.

Save most explanation and interpretation for the discussion section.

Tables

The table above is an example of a well-constructed table.

- The title is simple and clear.
- The column headings are accurate and contain the units.
- The uncluttered data are easy to read and understand without reference to the text.
- The data are sorted (after the reference compound) in decreasing value by the most important column \(V_{\text{max}}/K_m\).
- The absolute value of the reference compound is reported as a table footnote.
- The number of significant digits in the values does not exceed the precision of the determination.

Figures

The sample figure shown below exemplifies an easily understood figure.

- The purpose of the figure is readily discernible by visual inspection.
- The title of the figure is clear, simple, and relevant.
- The legend contains adequate information to understand the figure.
- The un-crowded figure contains adequate and balanced white space.
• The curves are labeled within the figure (if acceptable by the journal) to avoid the need to flip visually between the graphic and the legend.
• The curves don’t extend beyond the data points.
• The symbols clearly distinguish the curves.
• The axes are labeled clearly and have meaningful values with appropriate intervals.
• The text remained legible after photographic reduction.

Discussion

This section brings out the significance of your work and relates it to the literature (and to your introduction). Although a brief rehash of results may be appropriate, this is not the place to present results. Discuss, interpret, and comment on all significant findings and discrepancies, which are better discussed here than left as fodder for potential critics.

Your manuscript will be much easier to write and will read much better the first time if you take the time to do a "paper and pencil" preliminary outline of the points to be discussed. This approach keeps the manuscript flowing in a logical way and prevents rambling.

Readers tend to remember best what they read first and last. So cover the most important items first, and don’t try to bury items of doubt by saving them for last. End your discussion with a positive and optimistic conclusion concerning the most favorable aspect of your study.

Conclusion

This section should wrap up your findings and should indicate the future plans of the project. Refer to the downloaded article for a specific example of this section.

Experimental Section

The Experimental Section should begin with a paragraph that describes the make/model and parameters of all instrumentation used, how solvents were purified, column chromatography conditions, etc. The rest of this section should include an experimental procedure including the purification method and spectral data for each compound made. Too much detail can make this section excessively long. You should try to be concise, but complete.

Experimental Section Example:
First Paragraph
Tetrahydrofuran (THF) and diethyl ether (Et₂O) were purified by distillation from sodium/benzophenone under Ar immediately before use. Moisture- and oxygen-sensitive reactions were carried out in flame-
dried glassware under Ar. Solvents for chromatography (Et₂O, EtOAc, CH₂Cl₂, hexane) were distilled from CaH₂ prior to use. Flash chromatography was carried out under positive pressure using 32-63 μm silica gel and the indicated solvents. Melting points were uncorrected. Electron mass spectra (EIMS) were obtained at 50-70 eV. ESI spectra were generated in positive ion mode from an acetonitrile/water solution (50/50 v/v) containing 1% acetic acid. High-resolution (accurate mass) MALDI spectra were generated in reflector mode using a mixture of peptides and matrix cluster peaks as internal references. High-resolution chemical impact mass spectra (CI/MS) and FAB high-resolution mass spectra were obtained at the mass spectrometry laboratory at the University of Texas at Austin. Combustion analyses were performed by Midwest Microlab, Indianapolis, IN. ¹H and ¹³C NMR spectra are provided in the Supporting Information to establish purity for those compounds, which were not subject to combustion analyses.

Experimental Procedure Entry for a Compound
Tetra(2-aminoehtyl)methane (1) [Side Note: 1 is the number this compound appeared in the text] A solution of 3,3-bis(2-azidoethyl)pentane-1,5-diaide (9) (160 mg, 0.55 mmol) in 5 mL of absolute ethanol was combined with 10% palladium on carbon (16 mg, 0.1 mmol) in a hydrogenation vessel. The reaction mixture was hydrogenated at 40 psi hydrogen pressure at room temperature for 24 h. The suspension was filtered through Celite, and the filtrate was concentrated and dried in vacuo to give 94 mg of 1 as a viscous yellow oil (91%): IR (neat) 3295, 3385 cm⁻¹; ¹H NMR (200 MHz, CD₃OD) δ 1.39 (t, 8H), 2.63 (m, 8H); ¹³C NMR (50 MHz, CD₃OD) δ 36.9, 37.2, 41.2; MS (+ESI) m/z (relative intensity) 189 (MH⁺, 16); HRMS calcd for C₉H₂₄N₄ 189.2079, found 189.2086.

References or Literature Cited Section
Consult the particular journal's instructions to authors for the reference format or refer to your downloaded article and follow the format for referencing. Because this is an error-prone section, proofread and verify the references.

Acknowledgement
This section allows the authors to recognize any help received during their work. An example is given below.

Example: T. Spector is grateful to the many authors (himself included) whose literary errors inadvertently provided the basis of this article, and thanks the reviewers and editors who helped prevent this article from contributing to that collection. D. Porter, R. Miller, and J. Spector were especially helpful reviewers of earlier drafts.

Writing Style
Succinct Sentences
Well-constructed sentences are succinct. They are easy to read and understand. Succinct sentences unambiguously relay content and meaning. The five topics of this section describe methods for writing succinct sentences. You should try to construct the major part of manuscripts with succinct sentences. Less succinct sentences may be used for emphasis or to break up a string of succinct sentences that have become monotonous.

Tangible noun subjects
The following suggestion is probably the most important recommendation in this article. Use a tangible noun as the subject of the sentence¹. The key to writing a succinct sentence is to select the

¹ A tangible noun represents something that is touchable or concrete. The subject of a sentence does the action (active), is acted
Tangible noun subjects are meaningful subjects. They immediately direct the reader to the focus of the sentence. Whenever possible and appropriate, use a tangible noun as the subject of the sentence.

The following examples demonstrate the advantages of switching the subject (italicized) to a tangible noun. Notice the ease of reading and understanding the "succinct" sentences. In contrast, the subjects of the "original" sentences cause the reader to search for the intended meaning.

1. Original: In the rat, the metabolism of CX80 is characterized by the formation of three-polar compounds.
   Succinct: Rats metabolize CX80 to three polar compounds.

2. Original: Another issue that concerns the authors focuses on the interpretation of the in vitro data.
   Succinct: The authors are also concerned with the interpretation of the in vitro data.

3. Original: The modification of the method of Smith (ref) led to the generation of acceptable data.
   Succinct: Acceptable data were generated by modifying the method of Smith (ref).

4. Original: Elevation of intracellular ATP was observed following i.v. administration of compound Q.
   Succinct: Intracellular ATP was elevated following i.v. administration of compound Q.

Several words are giveaways for detecting convoluted sentences with weak subjects.

1. Excess prepositions: Note that three prepositions (In, of, and by) were eliminated by changing the above Example 1 to the succinct form.

2. It and there used as false subjects: Examples:
   (a) It is of concern to the authors....
   (b) There exists in the rat....

**Subject-Verb Location and Agreement**

People are easily lost in the forest between the subject and the verb. Keep your readers on track by placing the verb as close to the subject as possible. Gopen and Swan (1) discuss how intervening words interrupt the reader's expectations. In addition, subjects and verbs must agree in number (singular and plural forms). You can consult Dodd (2) for a discussion of this topic.

**Active/Passive Voice and First Person**

Although the active voice is more succinct than the passive voice (3), many scientists prefer the latter. They believe that the passive voice is more objective and, therefore, more suitable for scientific writing. I suggest using the active voice wherever appropriate. Using active voice in Example 1 under "Tangible noun subjects" added to the clarity of the sentence.

1. Nucleophiles generate peroxide radical. (Active)
2. Mice were treated with methotrexate. (Passive)

**Dangling and Misplaced Modifiers**

Make sure that modifiers actually modify what they are intended to modify. Otherwise, they may distort the meaning of a sentence. The following dangling participial phrases (italicized) lead the reader to wonder how the centrifuge turned the dial and who was incubated or was lying on the intestine.

1. Original: Turning the dial to 60,000 rpm, the centrifuge started.
   Corrected: The centrifuge was started by turning the dial to 60,000 rpm.

2. Original: Having incubated for 30 min at 37°C, we placed the vials on ice.
   Corrected: The vials were placed on ice after they had incubated for 30 min at 37°C.

3. Original: Lying on top of the intestine, you will perhaps make out a small transparent thread.
   Corrected: You may see a small transparent thread lying on top of the intestine.

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1. Example from Day (3).
The misplaced modifier and phrase (italicized) in these sentences substantially alter the intended meaning.

1. Original: The cells only secreted small amounts of peptide X.
   Corrected: The cells secreted only small amounts of peptide X

2. Original: A large mass of literature has accumulated on cell walls of staphlococci.
   Corrected: A large body of literature on cell walls of staphylococci has accumulated.

Wordiness
Words that don’t enhance content or meaning may bog down the reader. For example, the boldface words in the following sentence are either superfluous or redundant and should be deleted.

1. Original: We plan additional studies in the future in order to confirm previous experiments where replicate determinations consistently showed the pool sizes to essentially increase.
   Improved: We plan studies to confirm experiments where replicate determinations showed an increase in pool sizes.
   Better: We plan to confirm the experiments that repeatedly showed an increase in pool sizes.

The next sentence also becomes more readable as it is shortened. It is converted to a succinct sentence by replacing the false subject with a tangible noun and by using active instead of passive voice.

2. Original: It has been reported (ref) that hydroxyurea selectively decreases purine deoxynucleotide pools.
   Improved: Hydroxyurea was reported (ref) to selectively decrease purine deoxynucleotide pools.
   Better: Hydroxyurea selectively decreases purine deoxynucleotide pools (ref).

Verb Tense
Many authors struggle with the use of past and present verb tense. The rules, however, are simple.

1. Use the present tense to describe experiments and data that have been established and exist in the literature. E.g. Compound 6 is inefficiently degraded by guanosine hydrolase (ref).
2. Use the past tense to describe experiments and data of your present manuscript. E.g. Compound 6 was inefficiently degraded by guanosine hydrolase. (See the table on the next page.)

Word and Number Selection
The following items frequently surface as problems in scientific manuscripts.

Affect/Effect
Stick to the most common and least troublesome use of these words. Use affect as a verb meaning “to change or influence”, and effect as a noun meaning “a result or consequence”.

1. Excess acid will affect the yield.
2. He studied the effect of excess acid.

That/Which
People seem to be agreeing that that, which appears without a comma, should be used to introduce restrictive clauses, and that which, which appears with a comma, sets off nonrestrictive clauses. Strunk and White (5) advise to “go on a which hunt” to make articles more readable. The restrictive clause italicized in sentence 1 is necessary to the meaning of the sentence; whereas, the nonrestrictive clause underlined in Sentence 2 is not.
1. Only drugs that stop the virus from integrating into the human genome prevent chronic infections.

2. The mechanism, which may be concerted, is difficult to prove.

**In Vitro/In Vivo**

The term "in vitro" refers to experiments performed in an artificial environment with tissues, cells, organs, enzymes, fluids, etc. removed from living organisms. In vivo experiments are performed within living organisms. Thus, experiments with parasites and viruses in cultured cells are in vitro studies, or studies in culture, and differ from in vivo studies of infected animals or plants.

**Jargon**

Either carefully define or delete any laboratory terms that are not well established in the literature. Some examples of jargon follow. A correction appears in parentheses after the jargon.

1. Microsomal (endoplasmic reticulum) enzymes metabolize Compound Z in mice.
2. Reactions (reactants) were mixed in a glass vial.
3. Proteins were (protein concentration was) determined by the Bradford assay (ref).

**Auxiliary Verbs in Compound Sentences**

Auxiliary verbs should not be omitted when subjects change in compound sentences. The auxiliary verb "was" is needed in the second part of the following sentence to prevent the voice from switching from passive to active. Obviously, radioactivity cannot count. This type of error is commonly found in methods sections.

**Original:** Scintillation fluid was added and the radioactivity counted.
**Corrected:** Scintillation fluid was added and the radioactivity was counted.

**Significant Digits**

The number of significant digits in data should not exceed the precision of the determination. Because errors denote the magnitude of uncertainty, they should be presented with only one significant digit. Furthermore, this digit determines the least significant digit of the reported value. Thus, the leftmost place of the error determines the rightmost significant digit of the value. Accordingly, the $K_m$ for Compound 1 in the table is $15 \pm 1$ and not $15.32 \pm 1.27$, and the $K_m$ of Compound 6 is $120 \pm 10$, and not $122 \pm 11$.

<table>
<thead>
<tr>
<th>Substrate</th>
<th>$K_m \pm$ S.E. (µM)</th>
<th>$V_{max} \pm$ S.E. (µmol/min/unit)</th>
<th>$V_{max}/K_m$ (relative)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Guanosine*</td>
<td>$30 \pm 2$</td>
<td>$1.30 \pm 0.07$</td>
<td>100</td>
</tr>
<tr>
<td>Compound 1</td>
<td>$15 \pm 1$</td>
<td>$1.2 \pm 0.1$</td>
<td>190</td>
</tr>
<tr>
<td>Compound 2</td>
<td>$5 \pm 1$</td>
<td>$0.17 \pm 0.03$</td>
<td>78</td>
</tr>
<tr>
<td>Compound 3</td>
<td>$6 \pm 1$</td>
<td>$0.19 \pm 0.02$</td>
<td>73</td>
</tr>
<tr>
<td>Compound 4</td>
<td>$66 \pm 6$</td>
<td>$0.19 \pm 0.01$</td>
<td>6.6</td>
</tr>
<tr>
<td>Compound 5</td>
<td>$200 \pm 20$</td>
<td>$0.029 \pm 0.004$</td>
<td>0.33</td>
</tr>
<tr>
<td>Compound 6</td>
<td>$120 \pm 10$</td>
<td>$0.00097 \pm 0.00006$</td>
<td>0.019</td>
</tr>
</tbody>
</table>

* Reference substrate: specific activity was 450 mol/min/mg.

**Editing**

You are encouraged to have several colleagues comment on the content, construction, and style of your manuscript. Even accomplished writers benefit by critical reviews of their manuscripts. Peer reviewers are easy to find. Even some not-so-highly skilled writers may be clever reviewers. Remember to encourage your reviewers to be frank. Honesty may be more valuable than politeness.

The review process also allows you to distance yourself from your article. Writers often are too close
to their writing. You may not adequately describe complex material for the uninitiated, or you may not present a clear overall picture. Your colleagues' perspectives can be useful, but don't let too many cooks spoil the broth. Weigh all the opinions before making changes.

Literature Cited

“Precise Writing for a Precise Science”
Derived from Roger K. Bunting, Journal of Chemical Education • Vol.76 No.10 October 1999. 1408

Despite the pervasive necessity of effective communication skills in virtually any contemporary career endeavor, a good command of the tools of communication seems to have eluded a great many graduates of chemistry programs. Poor sentence construction and grammatical solecisms are all too common in both written and oral reports of scientific findings. The English language is the principal tool of modern scientific communication, and its effective use should be a goal of anyone preparing for a career in science.

Following is a collection of examples of familiar grammatical constructions, presented in scientific context that could be better phrased in accordance with the commentary that follows each.

Examples
The product has a melting point similar to benzophenone.

* A melting point in no way resembles a chemical compound, but it may resemble another compound's melting point. The sentence should read “... a melting point similar to that of benzophenone.”

Solubility was the principal criteria for choosing the nitrate salt.

* Criterion and phenomenon are two words of Greek origin often misused as their plurals.

The NMR spectra of compound 1 is shown in Figure 3.

* Spectrum (of Latin origin) is often casually replaced with its plural, spectra, by those who most often utilize spectroscopy.

The GC spectrum showed three peaks.

* Gas chromatography does not yield a spectrum, but a chromatogram. “The gas chromatogram showed three peaks.”

Pentaborane and ammonia were reacted at low temperature.

* Few besides chemists are brazen enough to use react as a transitive verb. The chemicals react, chemists don't react them. This usage is quite common, however, but it makes one wonder about the user's understanding of thermodynamics.

There was very little data to support the conclusion.

* In chemistry, data is still commonly used in the plural sense, and most chemists are careful to write data are instead of data is. The error is less obvious here, however, and this construction is often seen and heard. The sentence should read, "There were very few data". (As a simple check, if a sentence doesn't sound right when data is replaced by facts; it probably isn't correct.)

A simple IR spectrum infers a highly symmetrical structure.

* Infer means to draw a conclusion - the responsibility of the spectroscopist not the spectrum. One could say that the spectrum implies, but this too is a personification. A better sentence would be "A highly symmetrical structure can be inferred from a simple IR spectrum."

Compounds, which contain azido groups, are often explosive.

* The subordinate clause is "restrictive": that is, the sense of the sentence is changed if it is omitted. Restrictive clauses should begin with that. The sentence should read "Compounds that contain azido groups". Nonrestrictive clauses, which are not essential to the meaning of the sentence, begin with which and are set off with commas. The following is an example using a nonrestrictive clause: "Azido compounds, which contain the N₃ group, are often explosive."

We abandoned our work with nitrogen trichloride when we realized it was explosive.

* No chemist would misunderstand the intended meaning, but the sentence literally says that the work was explosive. The intended antecedent of the pronoun it is the object of the preposition with. The
sentence should read ".. when we realized the compound was explosive." Ambiguity from a casual use
of pronouns is all too common.

Applying VSEPR principles, the most likely structure was predicted to be planar.

Applying is a dangling participle. There is no noun that it could modify except structure, and the
structure clearly did not apply the principles. The sentence should be rephrased as follows: "By
application of VSEPR principles...". Equally poor are sentences like "The solution was filtered, resulting
in the recovery of the product." Which resulted should be used in place of resulting.

The ester dissolved in benzene was saponified.

This is a very poor construction because dissolved could be both be a verb or a participle, and the
sense is not dear until the reader reaches the end of the sentence. A better construction would be "The
ester was dissolved in benzene and saponified."

The crystals darkened, which indicated there had been decomposition.

The past perfect tense "had been" implies an event more remote than the past tense. Presumably the
crystals darkened at the same time that the decomposition occurred, not subsequent to it. Both verb
forms should be in the past tense, or both in the past perfect.

Submit your vitae and the names of three references.

Cats, superstition has it, are endowed with multiple lives, but not chemists. Here the plural vitae has
been used for the singular vita (Latin), which means life. In the above context, vita refers to a summary
of one’s professional life. This misuse is common in classified advertisements. Curriculum vitae,
however, is a proper singular form ("course of life"), declined according to the rules of Latin.

And what is the name of a reference? Probably the writer meant the names of three referees. A
citation lists a reference; a person consulted is a referee.

The coordination of metal ions in aqueous solution is generally octahedral.

A general rule is one that always applies. A better choice in the above sentence would be
usually or commonly or typically octahedral.

Ammonia readily complexes with many transition metals.

It's been said that any noun can be "verbed", and most verbs no doubt had their origins in nouns, but
complex is not yet widely accepted as having attained verb status. In the above sentence complexes
could be easily (and preferably) used as a noun: "Ammonia readily forms complexes".

A scientific report ought to be presented with a level of rigor and precision of the language
commensurate with those of the scientific findings. However, a rigid adherence to all grammatical "rules"
would render a writing devoid of style, and such adherence is by no means mandatory or even
recommended. But an understanding of the rules, their origins, and their contemporary interpretations
allows the informed writer or speaker to selectively use grammatical devices to his or her advantage, to
most effectively convey the information so that it will be received in the manner intended.

References
1985.

General Reviews