Style Guide for Chemistry Reports

“I don’t care what you know, I care what you said.”

Stephanie A. Myers

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INTRODUCTION

Every symposium I have attended on "What Industry wants from Chemistry Graduates" has emphasized the importance of communication skills, particularly writing skills.[1-6] Such skills are important enough that at the 1996 Biennial Conference on Chemical Education, a representative from Union Carbide said that his company taught its own technical writing course.[2] The company had even required some Ph.D.s to take it. The National Science Foundation's review of undergraduate education also emphasizes the need to teach science students communication skills.[7] To meet this demand, writing is a strong component of many advanced chemistry courses.

This guide is intended to be an "all-in-one" reference for the style of writing expected in the sciences with particular emphasis on analytical chemistry. My main sources are the *ACS Style Guide* edited by Janet Dodd[8] and the "Instructions to Authors" from *Analytical Chemistry*.[9] Chemists in fields other than analytical chemistry and those submitting to publications other than *Analytical Chemistry* may have slightly different requirements. Some variations from these two sources are mine--generally for simplicity. Other variations were suggested by professionals in the field,[10,11] especially the parts on memos and procedures. An attempt was made to design this document for easy reference. Suggestions for improvements would be appreciated.

The style used in scientific writing is slightly different than that in other fields. Since the subject matter tends to be difficult, clarity is very important. Conciseness is also valued. *Analytical Chemistry,* the most-read journal in analytical chemistry, limits its research articles to seven journal pages, adding that "Condensation of papers longer than this will normally be required by the Editor."[9] In addition, figures, tables and equations are often used by scientists to present large amounts of information in a concise form. Many readers prefer to only skim papers for relevant information. Therefore, use of such devices is encouraged so that useful information can be easily located. However, a traditional format for each of these has been developed and should be followed. No reader wants to waste time trying to figure out a different system. The appropriate formats are detailed in subsequent sections so that they can be referred to as needed.

Reports must always consider the audience. Unless the instructions dictate otherwise, this means your peers. Your peers should be considered people who are not in the class but have all the prerequisites so that they could have been.

In general, most scientific documents use an "impersonal" voice, which de-emphasizes the experimentalist. The logic of this is that good science should not depend on who conducted the experiment. The use of "I," "we" or substitution of a noun meaning the same thing generally indicates that this voice is not being used. Consider recasting such sentences into an "impersonal" form. For example, in the description of a procedure performed as part of an experiment, the same idea could be phrased as:

Measure the temperature. *(command)*
I measured the temperature. *(active, personal, couldn't anyone do it?)*
One should measure the temperature. *(active, personal, awkward)*
The temperature was measured. *(passive, best in this case)*

However, being impersonal does not always require a passive voice. For example,

The solution turned blue. *(active, impersonal)*
I saw the solution turn blue. *(active, personal)*

Beware, however, of making things more confusing. If clarity requires mention of the experimentalist, do so.[12] The use of impersonal constructions in scientific writing is becoming less rigid, so many forms are permitted. Consider the point you wish to make in deciding whether or not to cast the sentence in a different voice.

All papers, regardless of type, should be thoroughly proofread. Spell checking is far from sufficient. Not only are few scientific words actually in the data base, but a spell checker will not be able to determine if you mean “form” or “from,” “its” or “it’s” or many other problems. In fact, many PCs have an automatic spell checker set as a default. It is a good idea to turn this off, since it will change the spelling of many scientific words to something completely different. For example, it will change all the capitalizations in chemical formulas. Grammar checkers are also very undependable.

Not only should the paper be checked for punctuation, grammar and spelling errors, but also for clarity and accuracy. For example, a student claimed “to dissolve the solute in NaCl.”[13] However, I doubted that he was actually working with molten NaCl, as this implies. One strategy to check the accuracy of what you said (compared to what you meant) is to have someone read your paper to you. There are many other ways of proofreading, but rarely can you effectively proofread your own paper.

The importance of real proofreading (versus spell checking) can be illustrated with the following poem:

> I have a spelling checker
> It came with my PC;
> It plainly makes four my revue
> Mistakes I cannot sea.
> I’ve run this poem threw it,
> I’m sure your pleased to no
> It’s letter perfect in it’s weigh,
> My checker tolled me sew.[14]

MANUSCRIPT FORMAT

Lab reports and term papers should be submitted in manuscript form, which is easily proofread. This is also the format in which research papers are submitted to journals.

Manuscript Checklist

word processed on white 8½" X 11" paper
double spaced
one side only
use a standard font such as Times Roman or Courier, 10 or 12 pt
pages numbered (usually centered at the bottom of the page)
justified to the left margin
one inch margins on all sides
use standard typographical customs (see below)
all figures and tables cited in the text
figures and tables collected at end of paper
has title page

Some of the common typographical customs include using one space after most punctuation marks, one space before a left parenthesis and one after a right parenthesis (i.e., spaces on the outside but no spaces on the inside) and no spaces next to dashes and slashes.[15] Although Lindsell-Roberts suggests only one space after a period,[15] it is still common to space twice after a period, and this is acceptable.   Paragraphs are indented either 5 or 7 spaces, but consistently throughout the document.[15] In a double-spaced document there are no extra line spacings between paragraphs. If you wish to check more specific details, you should consult a typing text such a *Mastering Computer Typing* by Sheryl Lindsell-Roberts.[15]

TITLE PAGE

The two essential items in a title page are the title and the authorship. Other items may be added on request from the instructor/editor such as the class, instructor, and date submitted or due. These are optional unless specifically requested.

There are two ways to approach the title of a paper. The best choice depends on the situation. *Analytical Chemistry* recommends a title with high keyword content. Keywords are words that are likely to be used in a computer search for information on a particular topic. Good keywords include technique used, analyte, variables tested, matrix, etc. For example, "Determination of Detergent-Derived Fluorescent Whitening Agent Isomers in Lake Sediments and Surface Waters by Liquid Chromatography"[16] describes analyte, matrix and technique.

Alternately, a "catchy" title can grab the reader's interest and set a more relaxed tone. It is rather uncommon in reports of scientific results, but it has been used effectively. The disadvantage is that such titles tend to be low on keywords and can, therefore, be missed by people doing computer searches for information. An example of a catchy title is "Clarifying the Haze. Efflorescence on Works of Art."[17] Note that this title was used in the "A pages" of *Analytical Chemistry*. The A pages are read for general information unlike the more specific research articles.

The title should be centered on both the page and line. Don't forget to capitalize all the first word and all other words in a title except articles and prepositions. A larger size font may be used for the title, but it should not be in bold or italic type, nor should it be underlined.

Any person who makes a significant scientific contribution to the work reported in the paper and who shares responsibility and accountability for the results is considered as a coauthor of the paper and should be listed as such on the title page.[18] This would include any of your lab partners. Other contributions can be indicated in a footnote or an “acknowledgments” section. The person responsible for the manuscript is the “corresponding author” which can be designated with an asterisk after the name. (The meaning of the asterisk should be defined at the end of the title page.)

In a list of authors, the first name is considered the most prestigious position. When that work is referred to in subsequent papers, everyone other than the first author usually becomes “et al.” Thus, this position is usually given to either the person who did the most experiments or the most writing.

An Example of a Title Page

John Doe* and Jane Student
Instrumental Analysis
Dr. Myers

*corresponding author

ABBREVIATIONS, NUMBERS AND EQUATIONS

Abbreviations. Abbreviations should be used sparingly, although long names often repeated may be worth the trouble of using one. When used, an abbreviation must be defined at the first point of usage. For example, in a paper about liquid chromatography (LC) you may not wish to repeat "liquid chromatography" throughout the paper so you would use LC for all subsequent references. Some very common abbreviations do not have to be defined. These include chemical symbols and formulas, mathematical symbols and unit symbols (remember that metric unit symbols do not have periods). Other standard abbreviations are defined in the following box. Capitalization and periods (or lack thereof) can change the meaning of an abbreviation and should, therefore, be given particular attention.

Standard Abbreviations

i.e. = that is to say
e.g. = for example
ca. = about
et al. = and others
p = page
pp = pages
No. = number
Ed. = editor (Eds. is plural)
ed. = edition
Vol. = volume (Vols. is plural)

Numbers. Numbers are often used in scientific reports. Therefore, they also deserve some special attention.

Numbers Checklist

initial zero before a decimal
no spaces before or after decimals
exponents for numbers in scientific notation (i.e., 6.02×10^{23} not 6.02E23)
space between number and units except for %, $ and °
appropriate significant figures
report error if known
appropriate units

Equations. Equations may refer to either mathematical equations or chemical reactions. Complex chemical reactions or mechanisms (for example, organic reactions where structures need to be shown) can be represented as figures instead of equations. Figures are preferred for reactions which will not fit on one line.

When equations appear in the text, they should be given a line to themselves and numbered sequentially (as they appear) on the right, with their own numbering system. They may then be referred to in the text according to the number. For example, Beer's Law

$$A = \varepsilon bC \qquad (1)$$

where A is absorbance, ε is molar absorptivity ($M^{-1}\cdot cm^{-1}$), b is path length (cm) and C is concentration (M) would be called equation 1 in the subsequent text. Don't forget that <u>all</u> variables must be defined, preferably with units. Once defined, the definitions do not have to be repeated in subsequent equations.

Variables which have meaning (rather than generic "x"'s and "y"'s) should be used. For example, a calibration curve in a spectrophotometric experiment would be a variation of equation 1, but the experimental results can be reported as part of an equation

$$A = (13.6M^{-1})C \qquad (2)$$

However,

$$y = 13.6x \quad (3)$$

and then defining x and y as absorbance and concentration, respectively, is not appropriate.

Equations Checklist

equation on its own line
all equations numbered in order of appearance
all variables are defined, including units
the equation number appears in parenthesis on equation line
the equation number does not have parenthesis in text

TABLES

Tables are used to present a large amount of precise information or to show inter-relationships between data in a more easily conveyed form than if reported as text.[8] The text refers to a table in support of an argument. However, readers often refer to a table without reference to the text. Therefore, a table should contain enough information to stand on its own. For instance, the experimental data for a standardization of HCl is shown in Table I.

Because a table should stand alone, it needs to have a clear format. The table should be numbered (with Roman numerals) *and* have a brief title which describes its contents. Traditionally, columns refer back to the leftmost column.[8] The top of each column should have a heading. If appropriate, the heading should contain units. However, units alone are not the column heading. The units are generally in parentheses either next to or below the column heading. If all the data in a column is the same, it is not appropriate to report that as a separate column. Instead, that information is reported at the top, under the title, as "common data." (See volume of HCl in Table I.) If there is no data in most of the entries, that column should probably be deleted and replaced with a footnote.[8]

Anomalies, such as blank spots, explanations of abbreviations, experimental details which apply to only to one or two entries, etc., can be explained in table footnotes. Footnotes should appear as superscripted lower case letters. These footnotes are defined at the bottom of the table.

If the numbers reported in a table are especially large or small, the exponent part of scientific notation can be reported in the heading (as it is for volume of NaOH in Table I). Technically, the sign on the exponent in the heading should be opposite that of the number (e.g., if the actual value is 0.0050, then the heading should be “X 10^3" if 5.0 is the value in the table, since 0.0050 X 10^3 = 5.0). However, this rule is not strictly followed. It is usually obvious from the type of data which form the author has chosen to use.

In manuscripts, each table is on a separate page and collected, in order, after the reference section.

Table Checklist

complete in one page
numbered in order of appearance *in text* with Roman numeral
informative title
sufficient information to stand alone (without reference to text)
common data, if any, collected at top
    no columns contain all the same number
unusual entries are explained with footnote
detailed explanations are made in footnotes
footnotes are lower case letters
    alphabetical as they appear in table
    defined at the end of the table
column headings contain appropriate units
columns are aligned
    left, right, centered or by decimal

Table I. Titration of HCl with NaOH

concentration of NaOH = 0.1001 M[a]
volume of HCl = 50.00 mL

vol NaOH $\times 10^3$ (L)	conc HCl (M)
50.10	0.1003
50.05	0.1002
50.14	0.1004

average concentration of HCl = 0.1003 ± 0.0001 M

[a]Determined by standardization against potassium hydrogen phthalate.

FIGURES

Supplemental materials other than tables come under the title of "Figures." This includes graphs, block diagrams, photos, drawings, etc. You can show either a series of chemical structures and/or a mechanism containing many structures as a figure. However, simple chemical reactions should be "equations." Figures tend to be very powerful and should not be neglected. They are often used in oral reports as well as written reports.

Like tables, figures should be numbered in the order they appear in the text (but with Arabic numerals) and collected at the end. The numbering system is separate for figures, tables and equations. However, the types of figures are not differentiated within the category. For example, a block diagram might be Figure 1 and a graph, Figure 2. Like tables, figures must have informative titles. If appropriate, a caption can be used to explain or label details in the figure. The figure number, title, and caption are written together (in that order) either at the bottom of the figure or on a separate page of figure captions. (See Figure 1 for an example.)

Figure 1 is an example of a block diagram. A block diagram shows the relationship between different components of an instrument. Block diagrams are frequently used to describe the instrument used in an experiment. In general, the blocks are the same for all instruments of that type, but the specifics vary. For instance, the column in Figure 1 could be polar, nonpolar or ion-exchange. Under some circumstances, it may be appropriate to cite specifics down to the manufacturer, such as describing the experimental details in an oral report. Under other circumstances, such as describing the theory of operation, a more general description would be appropriate.

Figure 2 is an example of a graph created with Quattro Pro from data obtained by Instrumental Analysis students.[19] Graphs are very powerful descriptions of experimental trends. There are a variety of graphing programs available; some are easier to use than others. In addition, most spreadsheets have graphing capabilities. Using a spreadsheet to graph your results has the advantage of being readily available. However, most spreadsheets are designed for business applications rather than scientific ones. Therefore, the method is not intuitive and a good looking graph is difficult. (See Appendix I for suggesting on graphing using Excell.) Scientific spreadsheets/graphing programs are easier to use and more versatile. However, they tend to be less common and quite expensive.

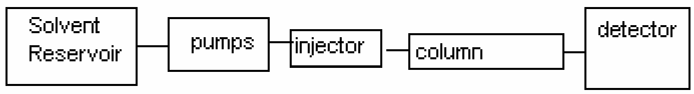
Graphs Checklist

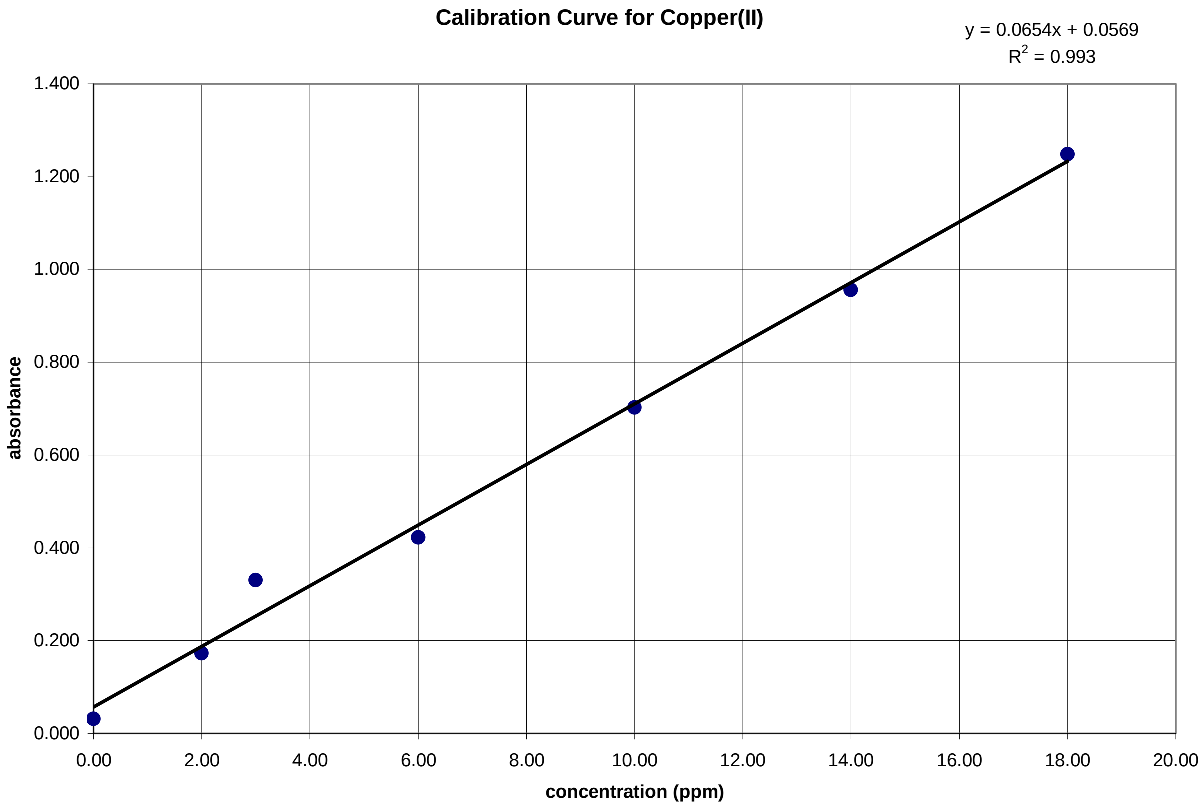
axes labeled, including units
ticks clear and at regular intervals
data points should be visible, but proportional with graph
    data points should refer to actual data not trend lines
ticks are labeled, and label numbers have appropriate significant figures
the trend line is appropriate
    (rarely is dot-to-dot appropriate; use a straight line or curve as suggested by data)

Figure Checklist

all figures are numbered with Arabic numerals (1,2,3...) in the order of appearance in text
all figures have a title
figure captions are either at the bottom of the figure or collected on a separate page
    these include figure number and title
any abbreviations used are explained in the figure caption
    (regardless of whether or not they are defined in the text)
figure stands alone without reference to the text

Figure 1. Block Diagram of Liquid Chromatograph




Calibration Curve for Copper(II)
y = 0.0654x + 0.0569
R2 = 0.993
1.400
1.200
1.000
0.800
0.600
0.400
0.200
0.000
absorbance
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
concentration (ppm)

REFERENCES

Any idea or statement which is not your own must be referenced; this includes direct quotations, summaries or paraphrases of someone else's opinions or ideas, data, statistics or other illustrative materials.[20, 21] However, common knowledge need not be referenced.[21] As a rule of thumb, any material which appears, unreferenced, in most textbooks on the subject can be considered common knowledge. *Failure to reference appropriately is plagiarism, which is immoral, illegal and ethically unacceptable in every profession.*

Rarely are direct quotes appropriate in scientific papers; a paraphrase in your own words is preferred. Exceptions to this are when who said it or how it was said is particularly important. As a rule of thumb, four or more consecutive words of someone else's writing should be considered a direct quote.[20] This rule must be used carefully and with common sense, since there are common three and four word phrases that are not appropriate to quote (e.g., United States of America). Short direct quotes can be bracketed by quotation marks, while longer quotes (more than 50 words) ought to be in a separate block, single spaced and indented on both sides.[8] An example of a long quote is the Augusta State University's College catalog's definition of plagiarism which states:

> Plagiarism is the failure to acknowledge indebtedness. It is always assumed that the written work offered for evaluation and credit is the student's own unless otherwise acknowledged. Such acknowledgment should occur whenever one quotes another person's actual works, whenever one appropriates another person's ideas, opinions or theories, even if they are paraphrased, and whenever one borrows facts, statistics or other illustrative material unless the information is common knowledge.[21]

The required style of referencing in most chemistry classes and by most chemistry journals is that of superscripted numbers, where the references are numbered consecutively in the order of appearance. Once a reference has been assigned a number, it retains that number throughout the paper. The number should appear in the logical place in the sentence, where reference to another person's work was made. For example, if the author's name is used in the text, the logical place is directly after the name. The references are then reported numerically in a separate section, titled "References."

A reference must contain all the information necessary for the reader to find the source referenced. The most common sources of information are books and journals; examples of how these can be referenced can be found in "guides to authors"[9] or a style guide[8] and in the reference section of this document. For books without editors, use the following format (note use of bold, italics and punctuation), skipping any item which does not apply.

Author 1; Author 2; etc. Chapter Title. *Book Title*, Edition number; Series Information; Publisher: Place of Publication, Year; Volume Number Pagination.

For example,

Emsley, J. Alcohol. *The Consumer's Good Chemical Guide*; W.H. Freeman: New York, 1994; pp 60-89.

Also see reference 12. For books with editors, the recommended format is

Author 1; Author 2 (of chapter); etc. Chapter Title. *Book Title*, Edition Number; Editor 1, Editor 2, etc., Eds.; Series Information; Publisher: Place of Publication, Year; Volume Number, pagination.

See reference 8 as an example. The format for scientific journals is

Author 1; Author 2; etc. Title of Article (optional). *Journal Abbreviation* **Year**, *Volume*, Inclusive pagination (or first page).

See references 16 and 17 as examples. For nonscientific magazines and newspapers, the format is

Author 1; Author 2; etc. Title of Article. *Title of Periodical*, Complete Date, Pagination.

For example,

Swearinger, R.; Ambrose, J. What a Dish! *Better Homes and Gardens*, September 2000, p 185.

Formats for less common types of references, such as government documents, can be found in the *ACS Style Guide.*[8, 22]

World Wide Web sites are becoming a common reference source. The method for citing electronic sources can be found in the second edition of the *ACS Style Guide*.[22] If possible, the reference should include the author's name, full title of the document, full http address (URL) and the date of the visit. All the information may not be available but as much as possible should be included. The document title is that which is found on the electronic site itself; the words "Home Page", or "database" can be added for clarification. If the URL does not fit on one line, it can be broken according to the following guidelines:

·break after an ampersand, slash or period, keeping two slashes together
·do not add a hyphen to the end of the line
·do not break after a hyphen to avoid confusion as to the hyphen's purpose

The general format is then

Author(if any). Title of Site. URL (accessed date).

Typical examples are:

ChemCenter Home Page. http://www.chemcenter.org (accessed Jan 1998).

ACSWeb. http://www.acs.org (accessed Feb 1998).

Rinaldi, A.H. The Net: User Guidelines and Netiquette-Index. http://www.fau.edu/~rinaldi/net (accessed May 1998).

Another good source of information is an interview with a person familiar with the subject. The interview can be conducted in person, over the phone or via email. Often the person will be able to suggest references. If interview information is used directly, it can be cited as a "personal communication" as is done in references 10 and 11.

Regardless of the source of references, it is important to evaluate their reliability. The most reliable sources are peer-reviewed books and journals. Anything printed by such publications has been reviewed for style and content by people who are working in the same field as the author. Non-peer reviewed printed material is less reliable but has at least had enough editorial review to have some credibility (if only to avoid a libel suit). On the other hand, there is no internal mechanism to evaluate Web-based sources, so it is totally the responsibility of the reader to decide on and to demonstrate the site's credibility. If a site fails to provide enough information to evaluate its reliability, it should not be used as a reference. The strength of your argument rests on the reliability of your sources.

Credibility Checklist

the sponsor of the publication
- is it a reputable group/person?
- is it likely to be biased about this information?
  (have a political or commercial agenda?)

do the authors give evidence of their credentials?
do the authors give evidence of their results?
- does the evidence support the results?

are the authors and the publication accessible?
how old is the information?
has the material been peer-reviewed?

Reference Checklist

references numbered in order of appearance in text
references cited as superscripts in text
references listed in numeric order at the end of the paper
- in a section titled "References"

references follow assigned format
- names, numbers and punctuation double-checked

reference section is double-spaced

LAB REPORTS

Lab reports are formal presentations of the results of your experiments. The model for lab reports is that of an *Analytical Chemistry* research article.[9] Lab reports are submitted in manuscript format and will contain at least some of the elements common to scientific papers, such as equations, figures, etc. These devices are very helpful to readers and should be used as necessary (rather than avoided because of extra work). These devices also allow information to be presented in a very concise manner. Journal space is very valuable and lab reports rarely make exciting reading. Therefore, shorter is better.

The format of these articles is very specific with sections having standard titles: Introduction, Experimental Section, Results and Discussion, References. Sections entitled “Conclusions” and “Acknowledgments” are optional and would appear between “Results and Discussion” and “References” if used. The titles of these sections are in all caps, left justified and given a line to themselves. The titles must be used as is without variation. For example, the first section is “Introduction” not “Theory” or “Purpose.” However, subheadings can be used within each section to clarify or organize the report. Subheadings are also in bold but appear at the beginning of a paragraph followed by a period, then the text. An explanation of the content of each section follows.

Introduction. The introduction of a report should contain the purpose of the report and the theory necessary to understand the method and the relevance of the results. In class assignments, it is easy to lose track of the purpose of the experiment in the midst of the purposes of the professor and the other requirements for the report. The purpose of the *experiment*, not the purpose of the professor or student is reported. An example of a purpose statement for an analytical experiment is “The concentration of iron in hematite was determined using standard addition and visible spectrophotometry.” Notice that the analyte and method are included, and the phrase “the purpose of my experiment” is not.

Experimental Section. This section describes how the experiment was conducted. It is not instructions for repeating the experiment, although it must contain sufficient information for the reader to do so. For example, the solutions used, including concentrations, should be included, but how the solutions were prepared should not be included unless the preparation was very unusual. Specialized apparatus (such as a liquid chromatograph) should be reported in detail, including manufacturer and model, but standard lab equipment (such as balances) should not. Any special safety precautions should also be mentioned in this section. Students tend to write too much rather than too little in this section.

Results and Discussion. Large amounts of data should be presented as a figure or table although simple findings may be presented solely in the text. Most of the text should consist of a discussion of these results, interpreting the relevance of the results. The purpose expressed in the introduction should be fulfilled here.

Conclusions. This section should only be used to interpret or unify results, but not to summarize information already given. Usually, this section will not be included.

Acknowledgments. Acknowledgments are rarely used in student lab reports. It is appropriate to acknowledge technical assistance, gifts, sources of special materials, financial support and auspices under which work was done in this section.

References. Refer to the previous section on references. If there is no information appropriate to reference, this section may be omitted.

Lab Report Checklist

appropriate sections are included

- introduction, experimental section, results and discussion required
- references, conclusions, acknowledgments optional

purpose

- described in introduction
- met in results and discussion or conclusions

standard format utilized for figures, tables, equations, etc.

TERM PAPERS

A term paper must be more than a collection of research articles. It is not sufficient to simply summarize the research, but it should also be evaluated and connected under a unifying theme. Typical themes in chemistry term papers show the relevance of the research to a broader problem, advance a particular position or predict a future trend. This theme ought to be presented early and obviously. Text which does not relate to this theme should not be included.

Term papers use manuscript format with the appropriate referencing style. (See those sections under Elements Common to Scientific Papers.)

Further guidelines depend on the professor.

ABSTRACTS

Abstracts are short summaries of a report. When a research article is submitted to a journal, it generally requires that an abstract of the article be submitted at the same time. Abstracts are also required of people presenting their research at a professional meeting.

Abstracts are very important, as they are the most widely read portion of a paper. Abstracts are not only published along with a paper, but also by abstracting services. Professional societies also publish abstracts of talks and posters given at meetings. In this case, the abstract often determines if someone will attend the presentation and may be the only hard copy retained with information from the presentation.

An abstract should describe the purpose of the research, principal results and conclusions.[9] This information must be presented clearly and concisely, since all abstracts have strict size limitations. For example, *Analytical Chemistry* limits abstracts to 80-200 words.[9] Abstracts for presentations generally have to fit a specific form and format. It is a stand-alone document and, therefore, should be written so that it can be read and useful without reference to the actual paper or presentation. In general, literature references are not included in the abstract.

The title of the abstract is also the title of the paper; a separate title page is not required. Information about the authors or the reference may also need to be included with the title, depending on the format requested by the editor.

"Quantitative Retention-Structure and Retention-Activity Relationship Studies of Local Anesthetics by Micellar Liquid Chromatography", Escuder-Gilabert, L.; Sagrado, S.; Villanueva-Camañas, R.M.; Medina-Hernández, M.J. *Anal. Chem.* **1998**, *70*, 28.

The retention of compounds in micellar liquid chromatography (MLC) is governed by hydrophobic and electrostatic forces. For ionic compounds, both interactions should be considered. The present report offers a novel retention model that includes the hydrophobicity of compounds and the molar fraction of the charged form of compounds and compares it with other previously reported models. High correlations between the logarithm of capacity factors and these structural parameters were obtained for local anesthetics with different degrees of ionization, using a nonionic surfactant solution as mobile phase. Modeling the retention of compounds as a function of physicochemical parameters and experimental variables is established by means of multiple linear regression. In addition, predictive models for estimating the hydrophobicity of local anesthetics is proposed. Finally, quantitative and qualitative retention-activity relationships in MLC are also investigated for these compounds. An excellent correlation between the capacity factors in MLC and the anesthetic potency of local anesthetics was obtained.

AN INVESTIGATION OF SURFACTANT EFFECTS ON BUFFERED SYSTEMS, Mary E. Newton and Stephanie A. Myers, Department of Chemistry and Physics, Augusta State University, Augusta, GA 30904. Surfactant solutions provide systems in which both hydrophobic and hydrophilic species are soluble and are, therefore, appealing as nontoxic and "green" solvents. However, due to the complexity of these systems, it is necessary to account for changes in reactivity due to the solvent itself. Therefore, the effects of surfactant on buffered systems were examined using potentiometric (pH electrode) and spectrophotometric (ultraviolet-visible) methods. The addition of surfactant does not affect potentiometric measurements, but the absorbance of the acidic form of bromocresol green increased (with corresponding decrease in basic form). This is attributed to an interaction of the acidic form of the indicator with the surfactant micelle altering the acid/base ratio rather than a change in pH.[23]

MEMOS

Memoranda are very common in all areas of the real (nonclassroom) world. The purpose of a memo is to communicate specific information quickly, generally within the workplace. Since most people are deluged with memos, shorter is always better. The subject and first line are very important, since that generally determines whether or not the rest of the memo will be read. The style is less formal than for a report. For example, this is a situation where first person reporting is appropriate. However, this is still a professional document and, therefore, a reflection of the professionalism of the writer. Informality is not an excuse for carelessness.

Memos are generally on letterhead or specific forms. The heading is very specific and must include to whom the memo is addressed, whom the memo is from, date and subject. Other than the heading, there is no opening or closing as are common in letters. The body of the text is separated by at least a double line from the heading.

Memos can be used to introduce other material. In this case, the additional material is called an "attachment." The existence of attachments is noted 2 or 3 lines after the body of the text, by typing "attachment" on a line by itself at the end of the page. (If there are x attachments, then "attachments (x)" is typed.) If a copy of the memo will be given to someone other than the one to whom it is addressed, this may be shown in the same area as attachments with "cc:" followed by the names of those receiving copies. The abbreviation "cc" originated from carbon copy.

<u>*Memo Checklist*</u>

Use “company” letterhead

Appropriate heading consisting of double spaced

- To:
- From:
- Date:
- Re: (or Subject:)

Memo should be single-spaced. Double spacing between paragraphs is ok.

one page or less

initial near your name on the “From:”

attachments and copies are noted at bottom

- if more than one attachment, designate the number in parenthesis
- list each person who gets a copy after “cc”

To: Dr. S.A. Myers

From: John Q. Student

Date: April 1, 1998

Re: Spectrophotometry results

There were 10.06±0.03 mg/L of Fe in sample #12. This was determined with the standard addition method.

I have found that standard addition is more practical than using a calibration curve for analyses of only one sample. Since standard addition only requires making one standard, while a calibration curve requires several, less time is required to perform the experiment.

The procedure for this analysis, the raw data and sample calculations for sample #12 are attached.

attachments (3)

cc: Jane Doe

PROCEDURES

Procedures are a written set of detailed instructions. Therefore, clarity is the most important element in this style of writing. To obtain sufficient clarity, such documents must consider both their audience and how instructions are generally read.

Experts don't bother to read the procedure, so it should be written for the novice. Therefore, most technical terms should be avoided or defined. To define terms, it is often useful to refer to a figure of the equipment so that the specific parts of it can be readily identified.

Procedures are read during the task and in short spurts so that each step can be performed immediately after reading that step *and* with minimum hesitation. No one actually reads (or at least remembers) all the instructions before starting. Therefore, only one instruction at a time should be given. A complex instruction will not be retained between the reading and the action. Additionally, explanations are generally not appropriate, since that is not the purpose of a procedure and will only distract from the instruction. If an explanation seems desirable, it could be included in a brief paragraph before the instructions start.

The instructions themselves should also be short and use the simplest possible style. This usually means the use of simple imperatives. An example of a simple imperative is "Close the door." This also avoids the awkwardness of gender-specific pronouns or the even more awkward avoidance of gender-specific pronouns. Addition of courtesy words ("please," "thank you," etc.) is also inappropriate, since they make the instructions longer without adding useful information.

Another consideration with procedures is the order. Since procedures are read as they are done, the order of the instructions must be the same as that of the task. Order can be emphasized by numbering the instructions. It may also be appropriate to separate the task into sections and give each section a heading. Words like “before” and “after” usually indicate that an instruction is out of order, indicating that an upcoming step should be done before the one being read. Instructions which are out of order can also be subtle. For example, if an instruction calls for using a 0.1 M solution, where was the previous step which called for making it? To avoid the latter situation, it is advantageous to have a list of needed materials at the beginning of the procedure.

Clarity also influences word choice. Many words are ambiguous in meaning. Relative terms like “large” or “enough” depend on the context and are not appropriate. For example, 10 μL is a large sample for capillary gas chromatography, but small for atomic absorption spectroscopy. It is better to give an actual value, even if it is approximate (say how approximate!). Even words like “replace” can be misinterpreted. Does this phrase mean to replace with a new part or the same one? Directional terms, like “front,” depend on the orientation of the instrument.

Avoiding explanation is not the same as avoiding warning. Warnings are important and should be placed in the position where the problem is likely to be encountered. Generally, these should be formatted slightly differently, so that they will be noticed and differentiated from the instructions. It can be appropriate to add a short explanation to emphasize the necessity of being careful. The more severe the consequences, the more the warning should be highlighted. Warnings can be highlighted by their introduction (“Note:” if less important, “Warning!” if more so) or by a change in typeface or position. Italics, underline, upper case letters and boldface type get progressively more forceful. These methods can also be used in combination. For example, compare the following warnings:

Do not let mixture reach 50°C.

Note: If the temperature reaches 50°C, cool the reaction or your product will be lost.

WARNING! AT TEMPERATURES ABOVE 50°C, MIXTURE WILL EXPLODE!

In these examples, notice how the explanation and the change of typeface makes the warning more forceful. The first might even be overlooked altogether since it blends in with the rest of the text.

Procedure Checklist one task per step short, simple imperative sentences no explanations as part of the procedure warnings highlighted order of procedure the same as the tasks technical, ambiguous and relative terms avoided

Procedure: Problem Solving[24]

1. Read the problem.

2. Read the problem again.

3. Write down what you hope is relevant information.

4. Draw a picture, make a list, or write an equation or formula to help you begin to understand the problem.

5. Try something.

6. Try something else.

7. See where this gets you.

8. Read the problem again.

9. Try something else.

10. See where this gets you.

11. Test intermediate results to see whether you are making any progress toward an answer.

12. Read problem again.

13. When appropriate, strike forehead and say “Son of a ...”

14. Write down an answer (not necessarily *the* answer).

15. Test the answer to see if it makes sense.

16. Start over if you have to, celebrate if you don’t.

POSTERS

Posters are used, as an alternative to an oral report, to present the results of research at professional meetings. A group of authors will display their poster on walls or bulletin boards as part of a "poster session." During the session, conference attendees wander through the posters. If a poster attracts their interest, the attendee will stop to examine the poster more closely and perhaps question the author who is required to be available (for that purpose) during designated times.

The author should be prepared for three types of people at a poster session. Most will give the poster only cursory attention and move on. They should be allowed to do so. Others may linger. It is appropriate to ask the lingerers "May I tell you about my poster (research)?" With an affirmative answer, the author responds with a prepared presentation which uses the poster as visual aids. This presentation is also useful for the attendee who asks the author, "Tell me about your work." Other attendees may already be familiar with the material and wish to ask more in-depth questions. It is appropriate to bring and refer to more detailed information than was presented in the poster itself. Regardless, it is important to be available to your audience during the designated time and not distracted by others' posters or by nonrelated conversations with friends.

Poster sessions allow in-depth discussions between author and audience which are not possible during an oral presentation. Thus, this is an excellent opportunity for getting help and insights form others working in fields similar to your own as well as more general networking. In addition, the poster itself is a finished project which is easily displayed later at your home institution.

The disadvantage of a poster session is the lack of a captive audience. Only people whose interest is caught (either by the topic or the poster itself) will pay more than cursory attention to your efforts. Also, the format prohibits detailed explanations (which are saved for the one-on-one discussions). Therefore, this format is best suited for information which can be displayed visually, with a minimum of explanation.

Since the audience must be attracted to the poster, it needs to be visually appealing. Whenever possible, the information should be displayed pictorially (like slides in an oral presentation), with most words acting as captions. Attendees of poster sessions will not read detailed explanations and, instead, ask the author if they wish more information. Nevertheless, your thesis or results should be obvious so that even a person who spends only a couple of minutes at your display can come away with the main point.

Posters are usually constructed in pieces which can then be assembled by attaching them to the display. It is traditional to frame each piece of the poster by gluing it to a larger piece of colored paper. The colors can then be used to section the poster or give it cohesiveness. Creative use of color and design can be used to capture the attendee's interest. However, the poster should be designed to capture interest in the *topic* of the poster, not the mental health of its author.

One essential piece of the poster is the title-author panel containing the poster title, authors and their affiliation (see "Title Page" section). This should be the largest panel on the poster. It is generally best to keep the other panels about letter size so that they may be easily transported (the title panel can consist of several pieces put together at the time of the session for transport purposes). All material should be easily read from a couple of feet away. Therefore, very large fonts should be used on the title-author panel, and 14 pt or greater fonts elsewhere. You can test the appearance of your poster by laying it out on the floor. If it looks good and you can read it while standing next to it, your poster is ready to go.

Poster Checklist
- stock oral presentation prepared
- each piece has about 1/2" colored border
- title-author panel
    - large, title, authors, affiliation
- visually appealing
    - neat, colorful, large print, minimal words
- thesis/conclusion obvious

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APPENDIX 1

Microsoft Excel 97–Graphing a straight line from your data

Data Input
Input x data in a column
Input y data in another column

Graphing
From options bar, choose *Insert* then *Chart* (Or click on "Chart Wizard" Icon)
"Chart Wizard" Menu will appear
Under "Standard Types," Choose (under "Chart type:") *XY (Scatter)*
Choose (under "Chart subtype:") the icon without anything connecting the points
Click on *Next>*
Under "Data Range", click in box to right of "Data range"
Highlight both x and y data columns
(note: may already be done, if so a dashed line flashes around data)
Be sure that under "series in:" there is a dot in the circle before "Columns"
(if not, click in that circle)
Click *Next>*
Under "Titles", click in box for "Chart title"
Type in name/title of graph
(e.g., Graph 1. Spectrophotometric Calibration Curve for Fe)
Click in box for "Value (X) Axis"
Type in title for your x-axis, include units
(e.g., concentration (ppm))
Click in box for "Value (Y) Axis"
Type in title for your y-axis, include units
(e.g. absorbance)
Click on "Legend"—which is at the top of the Chart Wizard window
Click on checkmark next to "Show legend", checkmark should disappear
Click on *Next>*
Under "Place Chart:", click on circle to let of "As new sheet", dot should appear in circle
Click on *Finish*

Your graph should appear on its own page.

Double click on the y-axis. "Format Axis" window appears
Click on "Number" at top Format Axis window
Under "Category" choose "number"
Input number of decimal places corresponding to the significant figures in your y-axis.
Click *ok*
Repeat for x-axis.
From option bar, choose *Chart* then *Add Trendline*
From "Add Trendline" window, under "Type", choose *Linear*
Click on "Options" at top of Add Trendline window
Click on box to left of "Display equation on chart", a checkmark appears (optional)
Click on box to left of "Display R-squared on chart", a checkmark appears (optional)
Click on *ok*
Save.

You may the modify graph to make it prettier or go directly to "Print."

Data Analysis

If doing this for the first time
From the option bar choose *Tools* then *Add-Ins*
Click on the box to the left of "Analysis Toolpack" (This may require that you insert the original CD.)
Click on *ok*

After "data analysis" has been set up...
From the option bar choose *Tools* then *Data Analysis*
scroll down to "Regression" and click on the word to highlight it
Click on *ok*

In the Regression window
Click in the white space next to "Input Y Range"
With mouse, highlight the y column of data
Click in white space next to "Input X Range"
With mouse, highlight the x column of data

Options:
If the first item in your column is not data, but the data description, click on "labels"
If you want the y-intercept to be zero rather than calculated, click on "constant is zero"
If you don't want the results on this on a different page, click in the circle to the left of "output range"
then click in the white space next to "output range" and use your mouse to highlight a cell for the upper left-hand corner of where you statistics will come out. Leave lots of space since it is 9 cells across and 18 cells down.

Interpreting your output...at least the results relevant to Dr. Myers
(note: some of the titles may be partially hidden because of the column size, you can expand by changing the column size at the top of the worksheet)

Under Regression Statistics
·The "R Square" value represents how linear your line is. The closer this value is to 1.0000, the more it is like a line than a curve. Rarely is any value less than 0.9 acceptable. If your value is less than 0.9, consider a different type of "fit"
·The "observations" value is the number of data points. You might find it useful to see if you actually included all your data or if you have more data than you want to count

Under the last section, where there are rows for "intercept" and "x variable"
·intercept refers to the y-intercept or b in the formula $y = mx+b$
the value for b is in the next column under the title "coefficient"
the error in this value is in the column after that under the title "standard errors"
·x variable refers to the slope or m in the formula $y = mx+b$
the value for m is in the column titled "coefficient"
the error in this value is in the column titled "standard errors"

ACKNOWLEDGMENTS

I would like to thank Karen Sisk for ideas, proofreading and saying "Yes, I think the project is worth doing." I would also like to thank Donna Hobbs, Tom Crute and Mary Newton for more proofreading, suggestions and some field testing of preliminary drafts.