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Academic English

Section: A BRIEF GUIDE TO WRITING IN CHEMISTRY

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APPENDIX 2:

A BRIEF GUIDE TO
WRITING IN CHEMISTRY

This document is a guide to assist students in chemistry courses with writing and formatting laboratory reports and research reports. An important goal of the Department is for our students to organize and communicate research results effectively and to write with acceptable scientific style. We hope that by providing many of the common stylistic, grammatical and organizational points in this single document, student can use this advice throughout their study of chemistry.

A. Formatting a Report

Layout. Use 12 point Times New Roman font and double spacing to allow space for comments and corrections. Number all pages, including those in appendices.

Organization. A standard lab report or research paper should be formatted with sections.

1. TITLE. List the title of the experiment or meaningful name for your research report. This is followed by your name and the date submitted. If you worked with partners, list their names next to yours, but put an asterisk after your name* to indicate that you wrote the report.

2. ABSTRACT. The abstract should be able to "stand alone." This means that someone should be able to read *only* your abstract and understand the basic nature of your report. For this reason, a good abstract clearly identifies the purpose of the experiment and the important results. Repeat: *a good abstract contains a summary of your results*.

Avoid pedagogical comments such as "this experiment helped us learn about the nature of chemical reactions" or "the goal of this experiment was to learn about dyes." Although those ARE important aspects and goals of the lab experience, the lab/research report should focus only on the data and results. Avoid starting your abstract with "The purpose of this experiment was..."

Background information on the theory or applications of your experiment belongs in the Introduction section. Avoid referencing any other sources or parts of the report, because the abstract should be able to "stand alone."

Be specific about what was done: name the reagents or types (not models) of instruments that were used, the products of a reaction, numerical values that were measured or calculated, etc. Avoid vague statements such as "a metal complex was prepared and the percent yield was calculated." A better abstract would read "hexaammine cobalt(III) chloride was prepared from cobalt (II) chloride, ammonia, ammonium chloride and hydrogen peroxide. The yield was 8.45 g (64 % based on cobalt)."

The best way to learn how to write a good abstract is to READ some published abstracts. These can be found in chemistry journals (for example, *The Journal of the American Chemical Society*) which are in the library.

TIP: When writing a full report, write the Abstract last.

3. INTRODUCTION. The introduction section explains to the reader what basic scientific question is being addressed. It includes general background material or a brief historical perspective on the topic being investigated. It presents brief summaries, with references, of previous work. An effective introduction funnels the reader from a larger area of research, through examples of progress in the field to a clear statement of the research problem or approach being addressed in the current report.

4. EXPERIMENTAL. This section includes a description of your experimental procedure, and names of instruments used. For lab courses, the procedure can simply reference the lab manual, listing any changes to the published procedure. DO NOT REWRITE THE LAB MANUAL. For advanced labs or independent research, the experimental section should provide all the necessary detail for someone to be able to reproduce your work. Often, an Experimental section is subdivided into **Materials** (sources and purity of reagents used), **Preparation of Compounds** (with procedure, and summary of characterization by NMR, IR, UV-Vis spectroscopy, melting point, chromatography, or elemental analysis) and **Instrumentation** (manufacturer, description of any adaptation or sample preparation) sections. Consult *JACS* to see examples of Experimental sections for various types of reports.

TIP: a good experimental section should allow another person, using what you have written and a lab manual, to completely reproduce what you did in the lab.

5. RESULTS & DISCUSSION. (may be single or separate sections) The Results should include a summary of your raw data (preferably in tabular form) and important observations. Do NOT include long tables of raw data; for those experiments simply present the results of your calculations. Calculations may be included in this section or in an Appendix, and a description of equations used in your calculations must be presented. Handwritten calculations are acceptable for lab reports.

A Discussion section should take the form of an analysis of your results. Comment on the purpose of the experiment. What do the results indicate? What are sources of error (experimental uncertainty/precision)? What additional experiments could help address any dangling ends? Do the results agree with what others have found? Do the results support a model or hypothesis? For some lab courses, you can use this section to answer any questions presented in the manual or in class. Although you should answer the questions in the lab manual, this section should have the style of flowing prose, not simply answers to numbered questions.

6. CONCLUSION. Summarize your results and discussion with a short conclusion that is more than simply a reiteration of your results. Phrase it in terms of the broader questions addressed in the Introduction.

7. REFERENCES. Citations of the literature used in the previous sections (see section F)

8. APPENDIX. Graphics may appear here, along with lengthy calculations or additional material not needed when reading through the report.

Graphics. Graphics include Tables, Figures, Schemes and chemical structures. Tables are columns of measured and/or calculated values or observations. All quantities should have units and be expressed using proper significant figures and scientific notation. Important experimental conditions should be listed as footnotes, especially when the table includes data obtained under different experimental conditions. Figures include: spectra, graphs, cartoons of experimental set-up or other drawings intended to show an *object*. Schemes include: reaction mechanisms, experimental flow charts or other drawings that are intended to show a *process*. All Tables, Figures and Schemes should be numbered sequentially and must be mentioned in the text. All graphics should be a full page in size and included at the end of the manuscript in the Appendix. Chemical structures can appear in the text and should be labeled with the same name, formula or compound number that appears in the text.

B. Sentence Structure and Writing Style

1. Beginning a sentence. Avoid beginning a sentence with a symbol, numeric value or equation.

incorrect: 315.6 mg of ammonium chloride was added to the solution, which was then heated to 50 °C.
correct: After the addition of 315.6 mg of ammonium chloride, the solution was heated to 50 °C.

incorrect: ν is both the vibrational frequency and the IR radiation frequency.
correct: The frequency ν refers to both the vibrational frequency and the frequency of IR radiation.

2. Dangling Modifiers and Illogical Construction. Check that a modifier phrase or the pronoun "it" actually refers to the intended subject. (see also: subject-verb agreement.)

incorrect: Being coated with grease, I cleaned the flask before adding reagents
was I coated with grease or was the flask?
correct: Because the flask was coated with grease, it was cleaned before...

incorrect: After transferring to a larger flask, the solution was heated to a boil.
did the solution transfer itself?
correct: The solution was transferred to a larger flask and heated to a boil.

incorrect: A diagram of the influenza virus is now available. To obtain it, contact the instructor. *The instructor is making the influenza virus available?*
correct: A diagram of the influenza virus is now available from the instructor.

incorrect: To prevent decomposition, the reaction flask must be purged of air.
does the flask want to prevent decomposition?
correct: To prevent decomposition, purge all air from the reaction flask.

3. Equations. Equations typically appear as a separate line from the text and are numbered sequentially throughout the manuscript. Equations can then be referred to by number.

example:
"The quenching rate constant can be calculated using the Stern-Volmer equation:

$$\Phi_0/\Phi_q = 1 + k_q\tau_0[Q] \qquad (2)$$

4. Hyphens. Hyphenate compound adjectives.

5-mL aliquots were added but, aliquots of 5 mL were added
crystal deposited from the slowly-cooled solution.

5. Spaces. There should be a space between a quantity and its units and between a quantity or word and subsequent parenthetical phrase.

6.626 J s
25.15 K = 298.15 °C
45 mL
456 nm (34,000 M^{-1} cm^{-1})

6. Personal Pronouns. By tradition, scientists avoid using the personal pronouns "I" and "we" and "you" in most technical communications. The use of third person instead of first person is preferred when reporting results. (see also: active voice)

first person: I heated the solution at 100 °C for 1 h. and I noticed that it turned blue.
third person: When heated at 100 °C for 1 h., the solution turned blue.

7. Pedagogical comments. Avoid including pedagogical comments in a report or scientific communication. Phrases such as "this experiment helped us learn about the nature of chemical reactions" or "the goal of this experiment was to learn about dyes" are addressing the process of learning not the science of the experiment. Although those ARE important aspects and goals of the lab experience, the lab report should focus only on the data and results.

Also, try to avoid starting your abstract with "The purpose of this experiment was..."

8. Personification. Molecules and equipment are not people, so do not personify them in your writing.

incorrect: Sugar really wants to dissolve in water.

correct: Sugar is very soluble in water.

incorrect: Sodium wants to lose one electron to form Na^+.
correct: Oxidation of Na to Na^+ is thermodynamically favorable.

incorrect: The spectrum shows two bands of equal intensity
correct: Two bands of equal intensity appear in the spectrum.

9. Plural nouns. "Data" is plural for "datum," "spectra" is plural for "spectrum," "phenomena" is plural for "phenomenon," and "formulae" is plural of "formula." The amount of chemical reagent is singular, so use the correct verb tense.

incorrect: Data was acquired and a spectra is in the appendix.
correct: Data were acquired and a spectrum is in the appendix

incorrect: While the solution boiled, 5.0 g of KBr were added.
correct: While the solution boiled, 5.0 g of KBr was added.

10. Prepositions. Don't forget "of" between quantities and substance name.

incorrect: "... and 10 mL MeOH was added."
correct: "... and 10 mL of MeOH was added."

11. Redundant or unnecessary phrases (pleonasm).

incorrect: A photon of light having a wavelength of 530 nm...
if not "of light," what was the photon made of?
correct: Light having a wavelength of 530 nm...

incorrect: In this experiment, aspirin was prepared from oil of wintergreen.
If not this experiment, then in which experiment?
correct: Aspirin was prepared from oil of wintergreen.

12. Subject-verb agreement. Are you stating that an inanimate object is drawing a conclusion, or suggesting a strange cause and effect? (see also: dangling modifers)

incorrect: The IR spectrum implies that water is in the aspirin sample. *(spectra don't imply, people do*)
correct: The presence of water in the aspirin sample is inferred from the IR spectrum.

incorrect: Water was present in the aspirin product because of the peak at 3200 cm^{-1} in the IR spectrum. (*the peak in the spectrum didn't cause water to be present*)
correct: The peak at 3200 cm^{-1} in the IR spectrum indicates that water was present in the aspirin product. (*water caused the peak in the spectrum)*

C. Verbs

1. Active voice. By avoiding personal pronouns, scientists often depend excessively on the passive voice, which can weaken the writing style. *When possible,* replace passive voice with active voice.

passive voice: A vapor was observed when the solution was heated.
active voice: A vapor formed above the hot solution.

passive voice: There was some solid that did not dissolve.
active voice: Some solid did not dissolve.

2. Subject-verb agreement. Based on whether the subject is singular or plural, use the correct verb tense. A quantity used is a singular subject, even when that quantity is in a plural form of units.

incorrect: 12 g **were** added
correct: 12 g **was** added

3. Verb tense. Past tense is used to describe a procedure that you followed in an experiment. Present tense is used to describe a scientific fact, such as the properties of a molecule.

examples: Hydrochloric acid was added to the flask slowly in order to prevent decomposition of the product. Hydrochloric acid is a caustic substance that must be used with caution.

4. "Verbing" a Noun. Don't turn nouns into verbs.

incorrect: ammonia complexes to cobalt ions
correct: ammonia forms complexes with cobalt ions.

incorrect: the mixture was centrifuged to separate the solid.
correct: The solid was separated from the mixture using a centrifuge.

incorrect: The solution was rotovapped to dryness
correct: The solvent was removed by rotary evaporation

D. Abbreviations, Formulae and Numerals

1. Standard Abbreviations. Use standard *JACS* abbreviations (note: not all journals use exactly the same abbreviations:

examples: mL = milliliter; μg = microgram; nM = nanomolar
h = hour; min = minute; s = second
K = degrees Kelvin, °C = degrees Celsius

2. Chemical Formulae. Use subscripts, superscripts, parentheses, and symbols appropriately in chemical formulae.

examples: $Cr^{3+}(aq)$
$K_2[PtCl_4]$
$[Ru(bpy)_3^{2+}](PF_6)_2$

3. Compound Numbers. Compounds can be numbered if repeated long compounds names become cumbersome. The number should be defined (usually in bold or underlined) somewhere early in the manuscript, often when it is first presented. The numbers should appear in parenthesizes when used as adjectives, but not when used as nouns.

example:

"Investigations into the fluorescence of 8-hydroxyquinoline (**1**), 4-iodo-8-hydroxyquinoline (**2**) and 2-methyl-4-iodo-8-hydroxyquinoline (**3**) are described in this paper. Recrystallization of **1** and **2** afforded analytically pure samples, but vacuum sublimation of the methyl derivative (**3**) was necessary to remove fluorescent impurities."

4. Decimal Places. For values less than unity, use a leading zero. Avoid writing values having too many zero; use scientific notation.

examples: "0.15 μL" not ".15 μL"
"2.3×10^{-5} M" not "0.000024 M"

5. Defining Abbreviations. Abbreviations for chemical compounds, ligand, instruments or methods should be defined in the text before using throughout the manuscript.

examples:

"The complex cation $Ru(bpy)_3^{2+}$, where bpy = 2,2'-bipyridine, is luminescent . . ."
"Surfactants such as sodium dodecyl sulfate (SDS) lead to lower drag . . ."
"Peptide structures were minimized using the empirical force filed (EFF) method."
"The American Chemical Society (ACS) sponsors two annual national meetings."

6. Organic Abbreviations. Standard organic abbreviations can be used in text and formulae.

examples:

Me = methyl
Et = ethyl
iPr = *iso*-propyl
tBu = *tert*-butyl
Ch – cyclohexyl

7. Reagents and Solvents. Use chemical formulae for standard reagents and solvents, but not when the name is shorter or more precise

examples:		
	NaOH (*aq*)	in place of "sodium hydroxide"
	H_2SO_4 (*aq*)	in place of "sulfuric acid"
	CH_2Cl_2	in place of "dichloromethane"
	"caffeine"	in place of $C_8H_{10}N_4O_2$

E. Chemical Terms and Expressions

1. Chemical names. The names of chemicals are not capitalized, unless they are trade names such as "Tylenol" or "Viagra."

incorrect: The reaction of aqueous Cobalt(II) with Aspirin was investigated.
correct: The reaction of aqueous cobalt(II) with aspirin was investigated.

2. Create. Chemistry involves "synthesizing" new compounds, "preparing" solutions, "characterizing" products. Avoid using phrases such as "products were *created*." Too divine.

3. Measurements. Spectra are measured "with" or "using" a spectrometer, not "on" a spectrometer (ouch!)

4. Machines. Spectrometers (UV-Vis, IR, NMR, etc.) are "instruments," not "machines."

5. React. As an intransitive verb, "react" should not have an object and should not have a passive voice. Chemical reagents react with each other, they are not reacted.

incorrect: "Potassium hydroxide and hydrochloric acid were reacted to produce water and potassium chloride."
correct: "The reaction of potassium hydroxide and hydrochloric acid produced water and potassium chloride."

6. Tested. A hypothesis can be "tested" and a student can be "tested." For most laboratory work, the terms "measured," "investigated," "determined," "calculated" or "obtained" often work better.

incorrect: The absorbance of the solution was tested using the UV-vis machine.
correct: The absorbance of the solution was measured using a UV-vis spectrophotometer.

F. References

There are numerous styles for formatting references. Unless otherwise instructed, citations should be formatted in the *JACS* style and appear as endnotes. Alternatively, article titles can also be included. Most important is to prepare citations with a uniform style.

Last name, initials; Last name, initials *Journal Title* **year**, *volume (issue)*, starting page.
or
Last name, initials; Last name, initials "Article Title" *Journal Title* **year**, *volume (issue)*, starting page.

examples:

Schlabach, M.; Limbach, H.-H.; Shu, A.; Bunnenberg, E.; Tolf, B.; Djerassi, C. *J. Am. Chem. Soc.* **1993**, *115*, 4554.

Additional Materials for Writing Lab/Research Reports

Davis, Martha *Scientific papers and presentations* San Diego : Academic Press, **1997**

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Eisenberg, Anne "Strategies five productive chemists use to handle the writing process." *J. Chem. Educ.* **1982,** *59,* 566.

Potera, Carol "The Basic Elements of Writing a Scientific Paper: The Art of Scientific Style" *J. Chem. Educ.* **1984,** *61,* 247.

Spector, Thomas "Writing a Scientific Manuscript: Highlights for Success" *J. Chem. Educ.* **1994,** *71,* 47.

> "To avoid criticism, do nothing, say nothing, be nothing."
> *-Elbert Hubbard*

Notes

Reference Note

Licensing Note

Preservation Notices

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