Chem 399
Professor Tessier
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Internship Reports

I. General comments

The major part of the grade for Chem 399 is determined by the internship report. The purpose of this handout is to provide guidance in how to write the report. If, after reading this handout, you still have unanswered questions, please contact Prof. Tessier (Email address = tessier@uakron.edu, phone = (330) 972-5304).

Department of Chemistry BS chemistry degree programs are certified by the American Chemical Society (ACS), the largest professional organization in the US for chemists. To maintain certification of our programs, students are expected to write a report that *at least* meets ACS guidelines. Though ACS does not provide specific guidelines for writing a report of an internship, ACS guidelines for preparing a research report should be applied as much as possible:
http://portal.acs.org/portal/fileFetch/C/CTP_005606/pdf/CTP_005606.pdf
In addition to these general directions, more specific directions are given below.

An important goal of the paper is to *convince the instructor that you learned some **chemistry** at a high enough level to receive 300-level college credit*. This means that the paper you submit for Chem 399 will NOT be the same as one you would submit as a report to company management or to publish the work. In these latter two situations, you are writing the report to specialists and there is no need to convince your reader that you have learned anything because it is assumed you know the background. In addition, the instructor for the course is not present when you do the internship work, so your writing must be more convincing than for Chem 499 or 497, courses that are done on site. Therefore, the Chem 399 report will contain more introductory material, such as on the chemistry you did, on the theories behind the work, and on the instruments you used. To help you determine what material to include, you may assume the reader has a bachelor's degree in chemistry (general knowledge in most topics) and is NOT a specialist in your field.

The instructor will help you write a good report. During the editing process, you may send the instructor report drafts via Email. However, corrections will NOT be sent to the student by Email. The student will pick up the corrected version from the instructor's office. *Printing of the **two copies** of final report is the responsibility of the student*.

II. Style of the internship report

II.A. General Comments on Style

The style of your writing should conform to that in *The ACS Style Guide* (2nd edition, Dodd, J. S., Ed., American Chemical Society: Washington, DC; 1997 or 3rd edition, Anne M. Coghill, A. M; Garson, L. R., eds., 2006) which is available at the Science and Engineering Library. ACS style is requested in order to get you used to the concept of writing in a particular style and because it is the most commonly accepted style. Lab reports for the Advanced Laboratory courses are written in ACS style or a similar one, so most Chem 399 students should already have some experience with it. If ACS style is not common in your area of work, then discuss this with the instructor *before you begin to write*. If your work is multidisciplinary, you may have to consult other style guides for the non-chemistry parts of the report.

II.B. Suggested organization of the report: A *suggested* organization for your paper is summarized below. The work you do in the internship may require that you modify this somewhat, especially if there are proprietary considerations. Prof. Tessier can provide guidance on this issue. It is suggested that you make an outline of your paper before you write. Good organization is essential to conveying your message.

✧ **Title page**: In a separate page, include the title of your internship, your name, the course number and the date.

✧ **Introduction**: An introduction to your project can include a historical perspective, background information or a discussion of relevance and applications. Also, keep in mind that the goal of the paper is to *convince the instructor that you learned some **chemistry** at a high enough level to receive 300-level college credit*. Here are a few examples:

Example internship dealing with paint. Define paint in terms of its major chemical components (including structure) and define the function of each component in the paint. Define important jargon in the field. If the component is acting as an emulsifyer, then indicate what an emulsifyer does. If you are studying a particular component in paint then introduce that component and provide more detailed information about the component.

Example internship dealing with lubricant oils and their impurities. What are the chemical structures of the lubricant oils that the company typically deals with? What are the structures of some the typical impurities in these oils? Explain the chemical and physical processes by which these impurities form. Explain the problems, especially chemical, caused by the impurities if they are present in the lubricating oil.

Example internship dealing with analysis of an industrial material. If you are using a particular technique to analyze the material, then provide background information on the method and how it can answer questions concerning the material. Industry often uses analyses that are defined by the American Society for Testing and Materials (ASTM) or other testing agency. Give the ASTM or other agency number and explain the chemistry and science behind the particular test.

If you are still unsure of which topics require introduction, ask the instructor. Note that in many cases, it may be best to interweave some introductory material in the Results and Discussion section rather than having all such material at the beginning.

✧ **Experimental section**:

The Experimental section is the most important part of your work and it is always separate from the Results and Discussion. Details of your work are given in this section. The explanations of your work (Results section) and its importance to chemistry and science (Discussion section) might be different if the experiment were reproduced at a different time. However, someone should be able to fully reproduce your Experimental section at any time, given access to the same materials, conditions, and instruments. Therefore, it is essential that you give enough details so that the work can be reproduced.

The Experimental section is usually divided into several parts. The first section of the Experimental is usually one to a few paragraphs that discuss the general methods and procedures used in the work. In these paragraphs, you can list the suppliers of the chemicals, purification methods used on the reagents and solvents, the

instruments and their settings, calibration methods for instruments. Provide references for standard techniques or calibration methods. If you use standard biochemistry kits such as the Quiagin Miniplasmid prep kit, mention them in the general Experimental paragraphs. Unless you make significant modifications in how the kit is used from the recommended protocol, there is no need to give the directions for kit use. Similarly, if you indicate that standard, Schlenk, synthetic techniques were used in the general paragraphs, there is no need indicate that a nitrogen or argon atmosphere was used in your description of each synthesis. However, it is important to indicate which gas was used in the general paragraphs because nitrogen reacts with some compounds. The name of companies or people who did some experiments or provided data should be included.

It is important that you be honest in writing the Experimental section. For example, consider the following two ways of describing that a precipitate forms in a reaction: “KI precipitated from the reaction” or “a colorless precipitate, presumably KI, formed”. Use the former if you did (at least) qualitative tests to assure that KI actually formed. If you just assumed KI formed because it is the expected product, then the latter phrasing is more honest. Another example occurs when solutions are exposed to vacuum in order to remove the solvent. You could say that “the solvent was removed under vacuum” but do you really know that solvent was the only component removed or that is was removed completely? Unless you actually check, it is more honest to say that “the volatile components were removed under vacuum”. In this case, it is important to specify in the introductory paragraphs of the Experimental the type of vacuum and, if possible, provide a measurement of the vacuum achieved. Fewer volatile components can be removed with an aspirator than with a vacuum pump or a vacuum-pump combined with a diffusion-pump. Such details may be important to someone trying to reproduce your work.

✧ **Results and Discussion section(s)**:

As indicated above, these sections deal with the explanations of your work (Results section) and its importance to chemistry and science (Discussion section). These two sections are often combined to avoid the redundancy that can occur when the Results and Discussion sections are separated. Summaries of the Results often must be interspersed within a separate Discussion section. In the Discussion, you should point out trends or inconsistencies in your work. If you used spectral methods to identify your compounds you should discuss which “peaks” (see discussion of this word below) were the most important for identifying your compounds. If your work involves a series of related compounds, you can discuss the trends in the spectral data for the series. You also should compare your results to those obtained by other researchers in your group or in different laboratories, or results obtained using different methods. If possible, discuss how your work has helped to move your field forward. You may also want to mention the potential practical applications of your work.

Results and Discussion sections can also be divided into subsections. In many cases, it may be useful to use different subdivisions in these sections than those used in the Experimental section. For example, in a synthetic paper, the Experimental section often is: compound **1** synthesis & spectral data, compound **2** synthesis and spectral data, etc. until all compounds are described. One could simply use this order for the Results and Discussion. Alternatively, the Results and Discussion could be divided in

sections such as: Synthesis, Physical Characterizations, NMR Spectroscopy, Mass Spectrometry, etc. These latter subsections more easily allow for comparisons to be made amongst the various compounds in the work.

In some internships, you may not be allowed to divulge the results you obtained because of secrecy concerns. In such cases, ask your supervisor if there are old results from previous workers that you can include instead. Alternatively, some companies place sample reports of analyses on their web sites. If you did those analyses as part of your internship, then you could use the sample report as the results and you would discuss the reports and and include them as appendices. (See below about appendices.)

✧ **Conclusions or Summary**:

End your paper with a Conclusion or Summary section. Such a section could include any of the following: a short summary of the key accomplishments, a list of unsolved problems, suggestions on how to solve these problems, or future directions you (or your company) will take in this line of work.

✧ **Acknowledgments**:

The Acknowledgements section is primarily used to say thank you. Often, it is used to thank a funding agency. In other cases, it can be used to thank a colleague, especially one who conducted an experiment whose results you used or who provided ideas for the project. This section is optional.

✧ **References and Notes**:

It is *required* that you consult the literature in writing your report. The following general sites of our libraries can help you begin your search.

- http://gozips.uakron.edu/~bolek/index.html
- http://gozips.uakron.edu/~bolek/chem.htm (may be phased out soon)
- http://www.uakron.edu/libraries/bierce_scitech/research_tools/subject-guide.dot?cat=631000&subj=Chemistry

Within those sites you will find links to many journals and e-books (many but not all *via* OhioLINK http://ebooks.ohiolink.edu/ebc-home/) and to important search engines such as Scifinder Scholar® or Reaxys® (formerly known as Gmelin, Beilstein, or Crossfire®). There are also links to more specific databases such as PubMed which is part of the National Institutes of Health and includes NCBI a biotechnology site (http://www.ncbi.nlm.nih.gov/). Many of these research databases provide output directly to programs that can manage your references, such as Endnote® or RefWorks®. The latter can be used by students at UA for free and can be reached from the topmost two web sites in this section. An advantage of using such a program is that the references can be automatically formatted in a variety of styles, including ACS style.

Though most useful sources of information can be reached from the above web sites, there are other sources that may be specific to your subfield of chemistry and may not be associated with the library web sites above. An important database that isn't reached from the above web sites is ExPASy (*Ex*pert *P*rotein *A*nalysis *Sy*stem, http://ca.expasy.org/) which is part of the Swiss institute of Bioinformatics. Several important structural databases are described in the section below entitled *Special directions for crystallographic figures*.

References and notes are to be numbered sequentially and listed at the *end* of your paper for this report. Most of your references should be to *reviewed* journals and

books from trusted publishing houses. Almost all material in our library and OhioLINK (http://www.ohiolink.edu/) is so. The manuals to instruments and software can also be used as references. Limit the number of references to web sites and personal communications because the material they contain is usually not checked or reviewed by anyone. If you must use web sites, then select sites that belong to reputable organizations or companies and include the date that you accessed them.

✧ **Appendix or Appendices**

An appendix (singular) or several appendices (plural) can be added to the report. *One appendix is required* in all reports and other appedices are optional.

ACS has mandated that all students not only receive training in safety but that they be tested on safety aspects or otherwise prove they know about safety. For this reason, the required appendix will include a discussion of the safety aspects of your project. In most cases, a 1-2 page safety appendix should suffice. This should include discussions on appropriate equipment required to handle the compounds in your work, the toxicity or radioactivity of your compounds, and the safety considerations in using an instrument such as an X-ray diffactometer, an NMR spectrometer, or a laser. You are still required to write this section even if your work is purely computational and you have never touched the compound that you are computing. Though you may include MSDS (material safety data sheet) in this appendix, this is NOT sufficient. Adding a MSDS to the report is not convincing proof that you actually read it or acted upon the information contained therin.

Examples of the types of information that can be included in the optional appendices are tables of data, spectra, sample mathematical calculations or a computer program. Number appendices if you use more than one. Separate each appendix from the rest of your report with a sheet that states the contents of the appendix. Three examples of what to write on the appendix separator sheet are shown below.

Appendix 1
Safety considerations

Appendix 2
X-ray crystallographic Tables for Compounds **3** and **5**

Appendix 3
Program for Modelling NMR Spectral Exchange Phenomena

Somewhere in your report, mention that the appendix exists and describe the information that can be found within it. Often a sentence is sufficient for each appendix. Captions should be used in the appendix material so the reader clearly understands how the materail relates to the rest of the report.

III. ACS Style details

The *ACS Style Guide* gives thousands of detailed suggestions for writing and it would be impossible for a student to learn them all at once. Therefore, a summary of the more important suggestions is given below.

✧ **Typing**:

Type your paper using one space after a comma, and one or two spaces after a period that ends a sentence. Indent five spaces at the start of a new paragraph. Use a space before and after an equal sign ("J = 3 Hz" rather than "J=3 Hz")

✧ **Tense and person**:

Most writing in the field of chemistry is done in the third person, which uses the chemical, reaction, instrument, analytical technique, etc. as the subject. Recently, it has become more acceptable to use the first person, using "I" or "we", in writing. However, it is difficult to teach when it is correct to use the first person as this varies with the subfield and it can appear arrogant if it is done too often or inappropriately. Therefore, avoid using "I" or "we", for this report. As your skills as a writer develop, you will learn when it is appropriate to use the first person in your field. The historical part of the Introduction section and all the Experimental section is written in the past. The Results and Discussion section can be written in a variety of tenses, as appropriate to the material. As much as possible, use the same tense throughout a paragraph and within a section.

✧ **Language**:

Use formal, standard, US English in the report. Be concise. Introductory phrases such as "It has been shown that" or "Note that" can usually be omitted from sentences without changing the meaning of the sentence. As shown in the table, some longer phrases can be shortened with no change in meaning. The *ACS Style Guide* includes many other examples.

Wordy	Less wordy
as well as	and
a number of	many several
blue in color	blue
rectangular in shape	rectangular
in spite of the fact that	although
due to the fact that	because
are known to be	are
at the present time	now currently
allowed to stir	stirred
allowed to reflux	refluxed

Avoid slang and the use of contractions. Brand names should be indicated with a ® symbol. Below are some examples of problem words.

- <u>While and since</u>: These two words are some of the most misused in scientific English. As stated in the *ACS Style Guide* (p. 46, 3rd ed.) these two words have "strong connotations of time". It is incorrect to use "while" or "since" to carry the meanings of "although", "because", or "whereas".
- <u>Data and datum</u>: Data is the *plural* and datum is the singular for these Latin based words. A very common mistake is to use a singular verb when the subject is the plural "data". Therefore, "the data *were* collected" is correct and "the data *was* collected" is incorrect.
- <u>Spectrum, spectra and spectroscopy</u>: The Latin-based word "spectrum" is the singular and "spectra" is the plural. In common speech, one can say "proton

NMR", "the proton NMR" or “by IR”. In formal writing, use "proton NMR *spectroscopy*" or "the proton NMR *spectrum*" or “by IR *spectroscopy*” (not in italics!).

- Peak: The word "peak" is used in common speech. In writing about NMR spectra, it is more appropriate to use "resonance" whereas in IR or UV-vis spectroscopy, it is more appropriate to use “absorbance”. In mass spectrometry, the use of the word peak is acceptable.
- Upfield, downfield, bathochromic, hypsochromic, hyperchromic, hypochromic, and red or blue shifted: There are a number of terms used to compare features in spectra. Different spectroscopies use different jargon. For example, do not compare NMR resonances by using the UV-vis jargon and vice-versa. In comparing two NMR signals, one resonance may be upfield (at lower chemical shift) or downfield (higher chemical shift) from another. In UV-vis spectrocopy and, less commonly, in IR spectrocopy, two signals can be compared by stating that one is shifted to the red (lower energy or frequency, higher wavelength, bathochromicly shifted) or blue (higher energy or frequency, lower wavelength, hypsochromicly shifted) of the other. Extinction coefficients of absorbances can also be compared: hyperchromic indicating an increase in extinction coefficient whereas hypochromic indicates a lowering. More commonly for IR spectra, different absorbances are simply indicated by stating that one is of higher or lower wavenumber or energy that the other, the two quantities being proportional to one another. For mass spectra, the jargon is simple, different peaks are of lower or higher mass from each other.
- Then, afterwards, firstly, secondly, etc: In chemistry writing, it is assumed that steps are given sequentially. Unless you stray from sequential listing of steps, words such as "then" or “afterwards” should be deleted from your writing.

✧ **Sentences and paragraphs**:

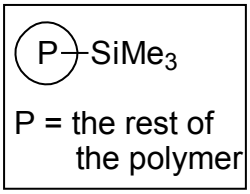
Use standard grammatical principles in writing sentences and paragraphs. A sentence should have a subject and a verb. Do not begin a sentence with a number. Use of “22 g of NaCl” at the beginning of a sentence is incorrect and should be replaced with “NaCl (22 g)” or “Twenty-two grams of NaCl”. The exception to this general rule is a number is part of the name of a compound. For example, the name “1,3-dimethylbenzene” can be used at the beginning of a sentence but you should capitalize the first letter (“1,3-Dimethylbenzene”). A paragraph should have at least two sentences. Indent new paragraphs. Use an introductory sentence at the beginning of each paragraph.

✧ **Abbreviations, acronyms and capitalization**:

It is important to use abbreviations, acronyms and capitalization correctly. Use standard abbreviations for units, elements, etc. (See *The ACS Style Guide*). The most common error in student reports is to use “l” rather than “L” for liter. The abbreviations of units are used in the singular and without a period (“mg” for milligrams but not “mgs” or “mg.”). Most units are separated by a space from the number (“22 mg” rather than “22mg”). As shown in italics in the following examples, capitalize the first letter of an element abbreviation but do not capitalize the element name.

the *Si-N* bond length vs. the *silicon-nitrogen* bond length
the *Si/C/N* ceramic vs. the *silicon-carbide-nitride* ceramic

The name of a compound is not capitalized unless it begins a sentence (see above). Define non-standard uses of abbreviations. For example, in figures that focus on the end group of the polymer, the letter P is often used to indicate the rest of the polymer. (See the drawing to the right of a $SiMe_3$ terminated polymer.) Such a non-standard usage should be defined because P is the accepted abbreviation for the element phosphorus. The name of a technique or instrument is not capitalized but the acronym is capitalized. An exception to this is when the name of a person (such as Overhauser below) is part of the phrase we use to define the technique or instrument.

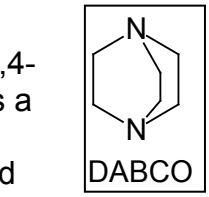


infrared spectroscopy vs. *IR* spectroscopy
nuclear Overhauser effect vs. *NOE*

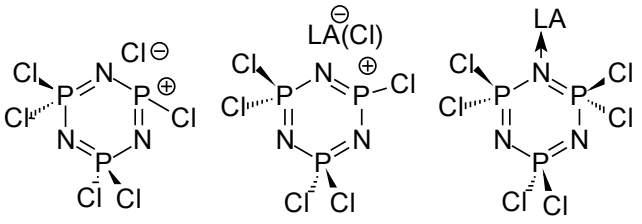
A common exception to capitalization rules is when an acronym is first defined, exemplified below for the acronym TBC. For emphasis, the letters that are used in the acronym can be capitalized.

1,2:5,6:9,10-TriBenzoCyclododeca-1,5,9-triene-3,7,11-triyne (TBC)

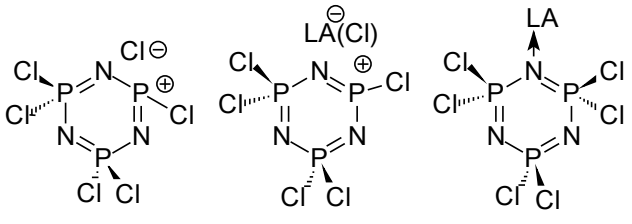
The names of compounds with complicated structures can be abbreviated as long as the abbreviation is standard (see *ACS Style Guide*) or the abbreviation is clearly defined by an IUPAC name (see TBC above) or a picture. For example, DABCO is a common (but not ACS accepted) abbreviation for 1,4-diazobicylo-2,2,2-octane (see drawing to the right). Usually, the drawing is a better way to specify a compound than by using a long IUPAC name. Alternatively, it may be useful to refer to compounds by numbers, assigned sequentially, using drawings or names, and with the compound number always **written in bold**. This is done correctly in this sentence for compounds **1**-**3**, in example Scheme 1, below. Compounds **1**-**3** can't be named easily because the Lewis acid is not specified, so the picture is necessary. Scheme 2 shows an alternative way of naming the three compounds. Such non-numerical acronyms are *not* written in bold font. Once you select a set of abbreviations, numbers or acronyms, don't name the compounds in other ways.



Scheme 1



Scheme 2



✧ **Equations, Figures, Schemes, Tables, Graphs, etc.**:

Use enough of these items to explain your work completely. Remember the old saying "a picture is worth a thousand words". Don't just tack such items to the end of your report. Point out and discuss ALL such items in your writing. Number these items sequentially. Keep a separate numbering system for each type of item. Tables, graphs, and figures should have a caption (as exemplified in Fig. 1 below). Equations are

usually not captioned and captioning is optional for schemes. A scheme differs from a chemical equation in that it can contain *two or more* equations or a very complex equation. Schemes also can be used to show a set of related equations, for example a mechanism, or a set of chemical structures, as in Scheme 1 and 2 above. A chemical or mathematical equation can interrupt a paragraph whereas figures, schemes and tables are placed after the end of the paragraph or are wrapped by the text. Make a clear separation between a figure, table or scheme, with its caption, and the rest of the report. An extra line or a box around the item usually suffices.

Frequently, tables, graphs and figures that are produced by an instrument are not properly formatted (i.e. subscripts and superscripts are not used), employ abbreviations that are non-standard, use non-standard English, fail to use Greek symbols properly, etc. If you include such material in your report, edit it if possible. Alternatively, use the caption to explain and correct the computer-generated figure. If there is no easy way to add a caption to a full-page plot or figure, you can simply use an extra page on which to write the caption. Place the page just before the item.

*It is expected that equations, figures, tables and schemes will be drawn **by you** using word processing, spreadsheet, chemical drawing or numerical equation programs*. A free chemical drawing program (Knowitall Academic Edition), which includes other useful programs, is available at: http://www.knowitall.com/academic/welcome.html. Line drawings and figures that display graphical data should employ carefully chosen font sizes, symbol sizes, and line thicknesses, and these should be consistent within a given figure. See the *ACS Style Guide* for examples of well drawn and poorly drawn figures.

✧ **Special directions for crystallographic figures**:

If you wish to include a drawing of a molecule that has been characterized by X-ray crystallography, you can do so in a manner that circumvents any plagiarism or copyright issues. Files that contain structural information can be downloaded from data bases of crystallographic data. With the use of certain programs to manipulate the 3-D structure, a different view of a molecule can be generated and saved. The new view of the molecule is not copyrighted and can be used in your document without fear of committing plagiarism. An example of such a drawing is shown in Figure 1.

There are several databases of structural information. For small organic and metallo-organic molecules (including a few inorganic molecules) the major structural database is the Cambridge Crystallographic Database (CCD, http://www.ccdc.cam.ac.uk/). CCD data are available in the CIF (Crystallographic Information File) format. CIFs are available as supporting information in some online journals. If the journal does not give the CIF file, it may be available it from CCD at: http://www.ccdc.cam.ac.uk/products/csd/request/. Requests for CIFs at CCD are usually granted within 1-2 days. The CIFs at CCD are free to academia. A free version of the program Mercury® from CCD is available at http://www.ccdc.cam.ac.uk/free_services/mercury/ to manipulate the structure and produce drawings. A similar

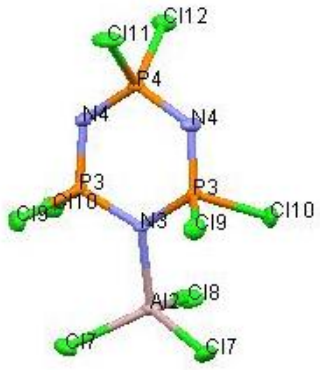


Figure 1. Example of a crystal structure plot drawn with the program Mercury® and the CIF from: Heston, A. J.; Panzner, M.; Youngs W. J.; Tessier, C. A. *Inorg. Chem.* **2005**, *44*, 6518-6520.

database for inorganic molecules, which also uses the CIF format, is the Inorganic Crystal Structure Database (http://cds.dl.ac.uk/cds/datasets/crys/icsd/llicsd.html). Unfortunately, free use of this database is restricted to European academics. For the CIFs of common molecules, the free database Reciprocal Net (http://www.reciprocalnet.org/) can be searched (funded by the National Science Foundation). The free Protein Data Bank (http://www.rcsb.org/pdb/home/home.do) can be searched by ligand, name, or PDB code. This database uses mmCIF files. Two programs can be used to manipulate the mmCIF files, pymol (http://www.pymol.org/) and jmol (http://jmol.sourceforge.net/). The faculty in the Libraries may be able to help you obtain CIFs in databases that charge for their services.

✧ **Photocopied, scanned or downloaded material**:

Photocopying, scanning, downloading *and similar* copying of material for inclusion in the report is strongly discouraged. It may be allowed only in cases of very complicated items. (Check with the instructor.) Part of the research experience is getting to use the appropriate drawing and spreadsheet programs to make your own equations, figures and schemes.

The copying of materials from journals and books is problematic because because such items are copyright protected. Web sites also may contain copyrighted information, *even if they contain no copyright notice*. (See: *ACS Style Guide*, 3rd ed. Chapter 7 for more about common misconceptions of web-based material.) The University does not allow such items to be included in graduate theses or dissertations without obtaining copyright permission because theses or dissertations are published on the web. If your report were to be published on the web, you would also be required to obtain copyright permission. Even if you will not be publishing the report, *it is still important to honestly indicate if you had NO significant part in creating the item*. Copyright laws make some allowances for the one-time use of copied material for educational purposes. **For this report, use a simple sentence such as "Taken from reference 2." in the caption of any item that you did not create to make it *absolutely clear* who created the item. Do this even if you don't know whether the material is copyrighted.** A reference number in the caption is NOT used in such cases because this is appropriate when **you created the item from material in a reference**.

There are grey areas where you might not know whether to use a superscripted reference number or a short sentence because your contribution to the creation of the item is only slight. Here are four example scenarios: 1) you download a figure and make a minor correction to it with a drawing program; 2) you load the structural coordinates you obtained from as supporting information in a publication into a drawing program, rotate the molecule, and generate the new drawing; 3) you combine two tables to generate a new table or 4) you used a drawing program to draw a figure that has some resemblance to one in the literature. In these instances, you can use captions such as the following, respectively:

-Scenario 1: "Scheme 3. The proposed mechanism of the polymerization of $[PCl_2N]_3$. Scheme modified from that in reference 3."

- Scenario 2: "Figure 6. Thermal ellipsoid plot of compound **7**. The figure was generated by using the program Mercury®

(http://www.ccdc.cam.ac.uk/free_services/mercury/) and the CIF in reference 6."

- Alternative for Scenario 2: "Figure 6. Thermal ellipsoid plot of compound **7**.[6,7]" (where one reference is to the publication and the other is to the program Mercury®.)
- Scenario 3: "Table 5. The rates of ethylene hydrogenation using commercial catalysts in aqueous solution. Combined table from those in references 3 and 5."
- Scenario 4: "Figure 2. The isomers of substituted trimeric phosphazenes.[3]"

Two possible captions are given for Scenario 2. In both, the program used to draw the figure is specified because different programs have different underlying assumptions. The use a superscripted reference in the caption (Alternative for Scenario 2 and Scenario 4) is *only* acceptable if *you created the item*. Use of sentences and captions as those given in the above scenarios *will help you avoid being accused of plagiarism!* More information on plagiarism can be found later in this handout.

✧ **Style of References and Notes**:

Reports will use ACS style for references, unless this mode is not used at all in your subfield. See your research advisor for advice on this point and for a style guide if non-ACS referencing is to be used. If you use a different referencing style, be consistent in it's use throughout the report.

ACS style for references varies with the subfield. However, the comments in this paragraph apply to all the styles. Use the same number for a particular reference throughout the paper. *Use the journal abbreviations recommended by ACS for references.* (See *The ACS Style Guide*.) In the references, list *all* authors and *all* editors. It is better to use inclusive pagination (both first and last page) rather than just listing the first page when citing a journal article. However, you should be consistent and use the same type of pagination for all journal references. A very common mistake is to omit the period at the end of a reference. *Note how punctuation and bold and italic fonts are used in the examples given separately below*, first for most subfields and then for biochemistry. The *ACS Style Guide* provides further examples on how to reference many sources of information including patents, web sites, on-line periodicals, CD-ROMs, government publications, unpublished material, and computer programs.

ACS Style for most subfields but not biochemistry

In ACS style for most fields except biochemistry, references are usually cited using a *superscripted number* as shown at the end of this sentence.[6] If possible, place the superscripted number *after* a punctuation mark such as a comma, colon or period rather than in the middle of a sentence or phrase. An example of how to cite several references at once is shown at the end of this sentence.[1-3,7,11-15] No spaces are used in the sequentially-listed, superscripted, reference numbers. Three examples of the proper way to reference various sources according to ACS Style are shown below, including pagination styles for books.

- ACS Style for a journal citation:

Heston, A. J.; Panzner, M.; Youngs, W. J.; Tessier, C. A. *Inorg. Chem.* **2005**, *44*, 6518-6520.

- ACS Style for a book without editors:

Shriver, D. F.; Atkins, P. W.; Langford, C. H. *Inorganic Chemistry;* W. H. Freeman: New York, 1990; Chapter 7. (Alternatively, the page numbers can be given rather than a chapter number.)

- ACS Style for an article within a book with editors:

Tessier, C.; Kennedy, V. O.; Zarate, E. A. In *Inorganic and Organometallic Oligomers and Polymers*; Harrod, J. F.; Laine, R. M., Eds.; Kluwer Academic: Dordrecht, The Netherlands, 1991; pp. 13-22.

ACS Style for biochemistry

It probably is not surprising that in an interdisciplinary field such as biochemistry, there are differences and more variety in ACS referencing styles. References are usually cited using an italicized number within parentheses as shown at the end of this sentence (*6*). Place the number *before* a punctuation mark such as a comma, colon or period rather than in the middle of a sentence or phrase. An example of how to cite several references at once is shown at the end of this sentence (*1-3, 7, 11-15*). Spaces are used in the sequentially-listed, italicized, reference numbers. Most ACS journals in biochemistry use styles similar to those shown above for the citation except that the title of the article or book chapter must be included. Interestingly, the most major journal in the subfield, *Biochemistry*, uses a different method than the other ACS biochemistry journals. These two major citing methods are shown with a few examples below. Ask your research supervisor which method to use. Be consistent and use only one of the two methods.

- ACS Style for a journal citation for most fields biochemistry journals:

Heston, A. J.; Panzner, M.; Youngs, W. J.; Tessier, C. A. Lewis Acid Adducts of $[PCl_2N]_3$. *Inorg. Chem.* **2005**, *44*, 6518-6520.

- ACS Style for a journal citation for the journal *Biochemistry*:

Heston, A. J.; Panzner, M.; Youngs, W. J.; Tessier, C. A. (2005) Lewis Acid Adducts of $[PCl_2N]_3$. *Inorg. Chem. 44*, 6518-6520.

- ACS Style for an article within a book with editors for the journal Biochemistry:

Tessier, C.; Kennedy, V. O.; Zarate, E. A. Silane dehydrocoupling reactions catalyzed by the late transition metals, in *Inorganic and Organometallic Oligomers and Polymers*; Harrod, J. F.; Laine, R. M., Eds.; Kluwer Academic: Dordrecht, The Netherlands, 1991; pp. 13-22.

- ACS Style for an article within a book with editors for the journal *Biochemistry*:

Tessier, C.; Kennedy, V. O.; Zarate, E. A. (1991) Silane dehydrocoupling reactions catalyzed by the late transition metals, in *Inorganic and Organometallic Oligomers and Polymers* (Harrod, J. F.; Laine, R. M., Eds.) pp. 13-22, Kluwer Academic, Dordrecht, The Netherlands.

✧ **Numbers and significant figures**:

Take care to use significant figures correctly. As the examples below show, it is important to understand the resolution and/or reproducibility of the instruments you use. With many instruments, there are a default set of parameters that most people use to obtain data. You should be aware of how many significant figures are allowed if you use the default parameters. Often, when the default parameters are used, the instrument provides data that have more figures than those that are significant. If you

use special parameters that allow for more significant figures, then you should list these parameters in the Experimental and mention the use of these parameters in the Results and Discussion. If the examples below do not include the instrument you are using, then ask your research advisor.

- Weighing: If the balance you used to weigh a chemical provided a weight of 2.41 g, then the number of moles should be given with three significant figures, the same number as the weight. Make sure that the molecular weight you use has at least as many significant figures as the weight of the chemical. Percent yields are usually given with no digits to the right of the decimal point, for example "85%" rather than "84.6%".
- IR spectra: On most IR spectrometers, the default resolution is 4 cm^{-1}. If you obtained the spectrum at 4 cm^{-1} resolution and the spectrum printout indicates the band occurs at 2122.35 cm^{-1}, then truncate and round the number to 2122 cm^{-1} because the other digits are not significant. You can use more digits if you set a higher resolution. However, doing so means that your spectrum will take longer to obtain. The default setting on most IR spectrometers for intensity measurements is the % transmittance scale. The absorbance scale is better for quantitative measurements or for making comparisons because it is directly proportional to concentration.
- NMR spectra: The reproducibility of NMR spectral data is related to the spectral window, to the referencing technique, to line-broadening processes and to other factors. For ^{1}H NMR spectra, which are usually run with a spectral window of about 10-15 ppm, the chemical shift is reproducible to two figures to the right of the decimal point, if you use the default settings. Therefore, the ^{1}H chemical shift of 8.327 ppm should be truncated to 8.33 ppm. For ^{13}C NMR spectra, a chemical shift of 8.327 ppm usually should be truncated to 8.3 ppm because the spectral window is usually set to ~200 ppm. For heavier nuclei, spectral windows can be in the thousands of ppms and even further truncation/rounding may be necessary. In the case of line broadening processes such as exchange, knowledge of the linewidth at half height can be used to further limit the number of significant figures. Truncate/round the numbers in *all* parts of the report. Use of an internal reference signal, such as from the solvent in your sample, gives more accurate chemical shifts than using an external reference. *The referencing method for all nuclei should be described in the Experimental section.*
- Single-crystal X-ray crystallography: Crystallographic measurements are usually followed by a number in parentheses, the estimated standard deviation (ESD). Make sure to report the ESDs of all distances and angles. Take ESDs into account when comparing two numbers. In X-ray crystallography, the rule of three ESDs is used. Two numbers are within experimental error if they are within three times the largest ESD. For example, the two bond distances 1.534(**1**) Å and 1.521(**1**) Å are different whereas 1.534(**1**) Å and 1.521(**9**) Å are experimentally *identical*.

IV. Ethical Concerns

It is expected that the report you write adhere to ethical guidelines. You should write about *your* work and not take the work of others as your own. In cases of collaboration, you should indicate which part of the work was done by someone else at

least once in the report. Be careful in overinterpreting data to make unwarranted conclusions. Below are links that deal with the general question of ethics in science.

ACS ethics page
http://portal.acs.org/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_TRANSITION_MAIN&node_id=1095&use_sec=false&sec_url_var=region1&__uuid=1929aae4-0e93-4709-bfaf-2bdea4bdd89e.

AAAS (American Association for the Advancement of Science) publication on ethics (one free download)
http://books.nap.edu/catalog.php?record_id=12192&utm_medium=etmail&utm_source=National%20Academies%20Press&utm_campaign=New+from+NAP+3.31.09&utm_content=Customer&utm_term=

Office of Research Integrity (part of the US Department of Human Services)
http://ori.dhhs.gov/

Plagiarism is a particularly important ethical concern in Chem 399 because a written report comprises such a large part of the grading. The paper you submit for Chem 399 will be checked for plagiarism. Plagiarism is considered a serious offense. Punishment for plagiarism can include expulsion from UA in serious cases. Plagiarism is not just a concern in academic courses as indicated by a number of recent articles in the prestigious journal *Science*.

- ✧ Couzin-Frankel, J.; Grom, J. *Science* **2009**, *324*, 1004-1007.
- ✧ Tara C. Long, T. C. Errami, M.; George, A. C.; Sun, Z.; Garner, H. R. *Science* **2009**, *323*, 1293-1294.
- ✧ Service, R. F. *Science* **2008**, *319*, 1170-1171.

Being accused of plagiarism in fulfilling the requirements of a course only affects **you** negatively. However, being accused of plagiarism in a publication or presentation can permanently damage your scientific career and those of your coworkers and can hurt the reputation of your University or place of employment. Some examples of plagiarism are listed below. In this list "written source" includes but is not limited to journals, books, web sites, newspapers, magazines, and work by another student.

- ✧ Copying of complete sentences and paragraphs from written sources
- ✧ Copying sentences from several different paragraphs of one or more written source and combining them to make a new paragraph
- ✧ Copying a sentence from a written source but modifying only one or two words
- ✧ Combining fragments of two or more sentences from written sources to make a new one
- ✧ Taking figures, schemes, tables, equations, etc. from a written source and not indicating that you took them

An important example where copying is acceptable is in the use of certain phrases for standard techniques or procedures. Terms or phrases such as "infra-red spectrum," "high pressure liquid chromatography," "Grignard reaction" can be copied. In fact, for some of these standard terms, it would be very confusing if you used different wording.

To avoid committing plagiarism, reference **all** ideas you have obtained from a book or journal and **write in your own words**. Before you write, turn your eyes away from the reference. Occasionally you may use someone else's words but this must be clearly indicated (with quotations or indented text for larger quotes) and referenced. Earlier pages in this handout describe the correct way of utilizing and referencing

material in which you have no or little part in creating (especially figures, tables, and schemes). UA provides information on academic honesty in the Undergraduate Bulletin and on the web sites for the Student Judicial Affairs Office and the Office of the General Counsel.

- ✧ http://www.uakron.edu/academics_majors/undergraduate_programs/ugrad.pdf (pp 7, 30, and 43)
- ✧ http://www.uakron.edu/studentlife/sja/index.php
- ✧ http://www.uakron.edu/ogc/staff/mallo.php

Another useful web site is: http://www.dartmouth.edu/~sources/about/what.html.
It is your responsibility to read and make sure you understand all guidelines on academic honesty given in this handout and at the above UA websites. If you do not understand, discuss this with the instructor **before** written assignments are due.