Chem 399
Professor Tessier
Updated August 1, 2008

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 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

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. A. 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 college credit*. If you are 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 (including solvents), the instruments and their settings, referencing or calibration methods for instruments, etc. Later sections of the Experimental are often divided into several logical subtopics.

In chemistry writing it is assumed that steps are given sequentially. Therefore, words such as "then" or “afterwards” should be deleted from most of your writing unless you stray from sequential listing of steps.

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? 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/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. You also should compare your results to those obtained by other researchers in your group or in different laboratories, to the results from other companies, or results obtained using different methods. If possible, discuss how your work has helped to move your field or your company's goals 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.

✧ **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.

✧ **References and Notes**:

It is *required* that you consult the literature in writing your report. You can use databases such as Scifinder Scholar®, Gmelin Crossfire® or Beilstein Crossfire® to find information about your topic. See Ann Bolek's (reference librarian for the physical sciences) website (http://gozips.uakron.edu/~bolek/index.html, click on databases) for a listing of databases and for information on how to uses them. Ann Bolek can provide help in the use of these databases. 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 Ann Bolek's web site. An advantage of using such a program is that the references can be automatically formatted in a variety of styles, including ACS style.

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.

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 two spaces after a period that ends a sentence. Indent five spaces at the start of a new paragraph.

✧ **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, except in the Introduction of the report where you describe the internship, avoid using “I” or “we”, in writing. 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 below, some longer phrases can be shortened.

a number of vs. many (or several)
blue in color vs. blue
rectangular in shape vs. rectangular
in spite of the fact that vs. although
due to the fact that vs. because
are known to be vs. are
at the present time vs. now (or currently)

The *ACS Style Guide* includes many other examples. Avoid slang and the use of contractions. Brand names should be indicated with a ® symbol. Below are some examples of problem words.

- Spectrum, spectra and spectroscopy: 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!).
- Data and datum: Data is the *plural* and datum is the singular. 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.
- Peak: The word "peak" is used in common speech. In writing about NMR spectra, it is more appropriate to call it a "resonance" whereas in IR or UV-vis spectroscopy, it is more appropriate to call a peak an “absorbance”.
- While and since: 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”.

✧ **Sentences and paragraphs**:

Use standard grammatical principles in writing sentences and paragraphs. A sentence should have a subject and a verb. A paragraph should have at least two sentences. Indent new paragraphs. Use an introductory sentence at the beginning of each paragraph. 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 the 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").

✧ **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 the following examples, capitalize the first letter of an element abbreviation but do not capitalize the element name.

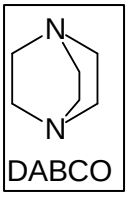
the Si-N bond length vs. the silicon- nitrogen bond

the Si/C/N ceramic vs. the silicon-carbide-nitride ceramic

Similarly, 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 is part of the phrase we use to define the technique or instrument.

infrared spectroscopy vs. IR spectroscopy

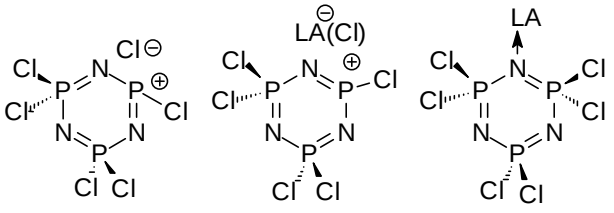
nuclear Overhauser effect vs. NOE



DABCO

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 a name or a picture. For example, DABCO is a common (but not ACS accepted) abbreviation for 1,4-diazobicylo-2,2,2-octane (see drawing). Usually, the drawing is a better way to specify a compound than by using a long 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.

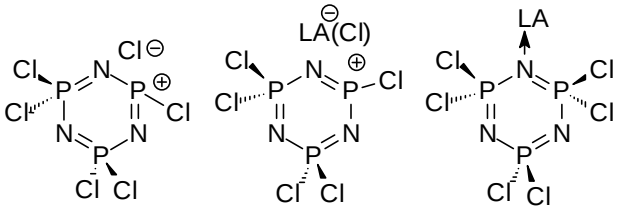
Scheme 1



1 **2** **3**

LA = Lewis acid

Scheme 2



T^+Cl^- $T^+[LA(Cl)]^-$ T(Cl)-LA

LA = Lewis acid

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

It is important to 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. There are several depositories of crystallographic data. Two major structural databases are the Cambridge Crystallographic Database (CCD, http://www.ccdc.cam.ac.uk/), which contains the structure of many small(er) molecules, and the Protein Data Bank (http://www.rcsb.org/pdb/home/home.do). These sites allow you to download the data file for the structure, use special programs to manipulate the 3-D structure, and print and save a particular view of the structure. Such a drawing is shown in Figure 1 above. For small molecules, use the free version of the program Mercury® from CCD, which is available at http://www.ccdc.cam.ac.uk/free_services/mercury/. This program uses CIFs (Crystallographic Information File).

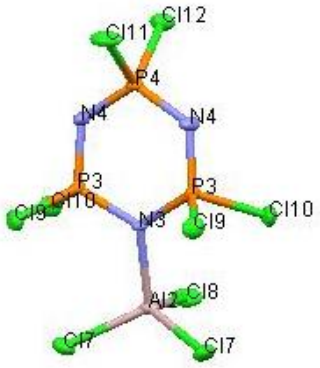


Figure 1. Example of a crystal structure plot drawn with the program Mercury® and the CIF from: Heston, A. J.; Panzner, M.; Youngs W. J.; Tessier, C. A. *Inorg. Chem.* **2005**, *44*, 6518-6520.

CIFs are available as supporting information in many 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. CIFs are free to academia. By using a CIF and Mercury® you can draw a different orientation of the molecule, one that is not copyrighted and can be used in your document without fear of committing plagiarism. (See below for more on these topics.) The Protein Database uses mmCIF files and has downloadable software to manipulate these files.

✧ **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 internship experience is getting to use the appropriate drawing and spreadsheet programs to make your own equations, figures and schemes. This is because such items are copyright protected. Note that the University does not allow such items to be included in graduate theses or dissertations without obtaining copyright permission because these works 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.* A simple sentence such as "Taken from reference 2." should be used in the caption of an item you did not create to make it *absolutely clear* who created the item. There are grey areas where you might not know whether to use a superscripted reference number, which is appropriate if you created the item, 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**:

In ACS style, references are cited using a *superscripted number*. 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. (If your area of chemistry uses a different referencing style, be consistent in it's use throughout the report.) Use the same number for a particular reference throughout the paper. *Use the abbreviations and style recommended by the American Chemical Society 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. Three examples of the proper way to reference various sources are shown below, including pagination styles for books. *Note how punctuation and bold and italic fonts are used in the examples.*

- **Journal**: Heston, A. J.; Panzner, M.; Youngs, W. J.; Tessier, C. A. *Inorg. Chem.* **2005**, *44*, 6518-6520.
- **Book without editors**: Shriver, D. F.; Atkins, P. W.; Langford, C. H. *Inorganic Chemistry;* W. H. Freeman: New York, 1990; Chapter 7.
- **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.

In the field of biochemistry, titles of the article are often included in the reference in ACS journals. Your supervisor may request you do this. The *ACS Style Guide* provides examples on how to reference other sources of information including patents, web sites, on-line periodicals, CD-ROMs, government publications, unpublished material, and computer programs.

✧ **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 supervisor.

- 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.
- 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.

- 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 data, which is usually run with a spectral window of about 10-15 ppm, the chemical shift is usually 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 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: Such crystallographic measurements are usually followed by a number in parentheses, the estimated standard deviation (ESD). Make sure to report the ESDs of 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. Plagiarism

Plagiarism is a particularly important ethical concern in Chem 399 because a written report comprises the largest 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 two articles in the prestigious journal *Science* (Xiguang, L.; Lei, X. *Science* **1996**, 274, 337 and Marshall, E. *Science* **1998**, 279, 473.). 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/docs/ugrad.pdf (pp 7, 30, and 43)
- ✧ http://www.uakron.edu/studentlife/sja/index.php
- ✧ http://www.uakron.edu/ogc/PreventiveLvaw/plagiarism.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.