Tools and Applications in Chemistry (CHEM4910L)
Spring 2018

Instructors:

Dr. V. Geisler TLC 2120 vgeisler@westga.edu (678) 839-6025 **Office Hours:** M 1-4, W 1-2 T, R 10-12:15	Dr. F. Khan TLC 2117 fkhan@westga.edu (678) 839-6027 **Office Hours:** M, W: 10:45 am - 12:00 pm W: 2:00 – 3:45 pm T:9:30 – 11:00 am; 12:00 – 2:00 pm R:9:30 – 10:45 am; 1:00 – 2:00 pm	Dr. S. Slattery TLC 2128 sslatt@westga.edu (678) 839-6027 **Office Hours:** MW 1-6

Schedule: Tuesday and Thursday 2:00 – 5:00 pm

Classroom: TLC 3115 (Analytical Lab) or 2105 (Lecture classroom)

Course Material:

- Permanent Bound Laboratory Notebook (not spiral-bound)
- Safety Glasses must be worn at all times in the laboratory and can be purchased from the Chemistry Department ($5).

Grading:

Organic Report	10%
Instrumentation Reports	20%
Experimental Design Report	8%
Applications of Chemistry Report (field trips)	3%
Inorganic Reports	20%
Oral Research Proposal	5%
Oral Research Presentation	10%
Final Research Paper	20%
Laboratory Notebook	4%

Grading Scale: 90-100 A, 80-89 B, 70-79 C, 60-69 D, <59 F

Learning Outcomes:

1. Design and carry out authentic experimental protocol for scientific investigations.
2. Learn to use chemical methods and instrumentation.
3. Write and revise formal lab reports containing abstract, introduction, experimental, results, and discussion sections and be able to appropriately prepare figures, tables, reaction schemes, and a bibliography according to the format commonly used in chemistry journals.
4. Utilize manual and on-line literature searching to retrieve information on:
    a. Chemical and physical properties of substances
    b. References for chemical reactions
    c. Recent review articles on a subject plus complete bibliography of an author
5. Explain the process of the peer review system
6. Prepare and present a well-reasoned oral presentation on a scientific topic:
7. Compose a well-reasoned response to an ethical problem in scientific research.

Tardiness / Missed Lab: Lab attendance is mandatory. At the beginning of each laboratory we will discuss theory and principles related to the laboratory. Lateness will be penalized by deduction of points from your lab report. Do not leave the lab early unless your task is completed. You will earn the grade of zero for any missed lab.

Policies: Read all laboratory material before coming to lab. You are responsible for the cleanliness of the laboratory. You must clean all apparatus at the end of each experiment. Borrowed equipment or chemicals should be returned by the end of each lab. All chemical waste should be disposed properly. Special care should be made to keep the area around the balances free of spills. Safety goggles and closed-toe shoes must be worn at all time during lab activities.

Course Den: Course Den will be utilized to post the syllabus and handouts, as well as grades. You will turn in lab reports via the Dropbox in CouseDen and Turnitin will be used to assess plagiarism. Announcements may also be made via this site. Please check this site between classes.

Academic Misconduct: Honesty in reporting results is one of the essential characteristics of your laboratory work. You will be more severely penalized for misrepresenting results than for honestly reporting "poor" results. Copying any part of journal articles, books, or website without proper citation are considered academic misconduct and will be penalized to the fullest extent possible**. Do not copy any part of other people's lab reports, including your lab partner's (this applies to all parts of reports, including contents, figures and tables). Even if you worked with a lab partner, you must write your report individually.**

Discipline-Specific Writing: This course has been designated as a Discipline-Specific Writing (DSW) course. The writing components of this course are essential part of this course and are designed to train you in scientific writing. This will entail writing in your laboratory notebook and laboratory reports. Your laboratory notebook will be a place for planning, calculation, procedure and record of all raw data and observation. Detailed instruction will be given in class. Your laboratory reports must follow appropriate scientific writing format and some may require rewrites to improve your writing of scientific papers. See attached guideline for the format. We encourage students to turn in drafts of their lab reports before the due date to get feedback before the final report is due. A minimum of 4,000 words across all writing assignments, not including revisions, is required for each DSW course.

Lab Notebook: You are expected to keep an up-to-date hand-written original record of all experiments you perform. All records must be entered directly into the notebook in non-erasable ink. **The notebook must be up to date all the time. Make all entries on the same day of the experiment and as you perform the experiment.**

As you carry out your experiments, you will record the procedure that you actually performed (written in the past tense and in the third person), observation, physical data (e.g. melting point) and types of spectra collected (e.g. ^{1}H NMR in DMSO-d_6). The spectra themselves will most likely be attached to your reports, so they do not have to be included in the notebook.

Reports: You will be given a basic outline of each experiment or project and specific goals to achieve. After completion of each project, you are expected to write a comprehensive report in a proper, scientific format, following the guidelines (see below). **Remember, writing a report is individual work and you may never copy or share ANY part of other people's reports, including drawings and tables,** even of your lab partner's. The only part you would share with your partner is the raw data, which is to be recorded in each individual's lab notebook. **The reports must be turned in electronically to CourseDen Dropbox.** Only the **.doc** or **.docx** files are acceptable.

Report Due*:* The report should be submitted on the due date indicated in the syllabus, or as announced in class. There will be a deduction of 5% (5 points) per day for late submissions.

Project: The Senior Project is the climax of the course it is a significant piece of work, designed by the student that demonstrates the ability to work independently, to analyze and synthesize information, and to write and speak persuasively. After the instructors give their research presentations, you will each be assigned one of class instructors to be your research mentor. **You will then generate research questions, carry out literature search, submit a research question and an experimental plan to address it, backed by the literature**. This research plan must be approved by the research mentor. Your senior project will culminate in an oral presentation and final formal report. The formal report must include the following sections: Abstract, Introduction, Experimental, Results, Discussion (Results and Discussion can be combined), and References.

Oral Presentation: See the webpages below to learn to make effective presentation.

https://acscareers.wordpress.com/2012/09/03/are-your-presentations-perfect/

http://acscareers.wordpress.com/2010/11/29/oral-presentations-preparation-is-everything/

Tentative Schedule for Spring 2017

Week #	Tuesday	Thursday
1	**Jan 9** – Syllabus, Safety Keeping a lab notebook, Communicating scientific work, SciFinder and ChemDraw (ACS room)	**Jan 11** – Organic – Geisler
2	**Jan 16** – Organic – Geisler	**Jan 18** – Organic - Geisler
3	**Jan 23** – Instrumental introduction Caffeine solutions DUE – *Organic* (draft report)	**Jan 25** - Peer review of draft report Caffeine solutions
4	**Jan 30** – Instrumentation – Khan/Geisler DUE – *Organic* (final report)	**Feb 1** – Instrumentation – Khan/Geisler DUE – *Instrumentation 1* (draft report)
5	**Feb 6** – Instrumentation – Khan/Geisler	**Feb 8** – Instrumentation – Khan/Geisler Experimental design introduction DUE – *Instrumentation 1* (final report) DUE – *Instrumentation 2* (draft report
6	**Feb 13** - Experimental design - Geisler DUE – *Instrumentation 3* (draft report)	**Feb 15** – Experimental design - Geisler DUE – *Instrumentation 2* (final report)
7	**Feb 20** – Applications of Chemistry: Water treatment plant (field trip) Faculty research project presentations DUE – *Instrumentation 3* (final report)	**Feb 22** – Applications of Chemistry: Southwire (field trip) Faculty research project presentations DUE – *Experimental design* (draft report)
8	**Feb 27** – Inorganic 1- Slattery DUE – *Application of Chemistry* (final report only) **DUE – Research project preference**	**March 1** – Inorganic 1- Slattery DUE – *Experimental design* (final report)
9	**March 6** – Inorganic 2- Slattery DUE – *Inorganic 1* (draft report)	**March 8** – Inorganic 2- Slattery **DUE – Research plan approval by mentor**
10	**March 13** – Inorganic 2- Slattery DUE – *Inorganic 1* (final report)	**March 15** – Inorganic 2- Slattery DUE **- Research question, research plan, literature reference** – presentation if time
	March 20 Spring Break	**March 22** Spring Break
11	**March 27 – Research project** DUE – *Inorganic 2* (draft report)	**March 29 – Research project**
12	**April 3 – Scholar's Day No class**	**April 5 – Research project** DUE – Inorganic 2 (final report)
13	**April 10 – Research project**	**April 12 – Research project** **DUE – Orally summarize the research progress to your faculty mentor**
14	**April 17 – Research project** DUE – **Research partial write up** (Introduction, part of Experimental Procedure, part of Results and Discussion)	**April 19 – Research project**
15	**April 24 – STUDENT RESEARCH PRESENTATION**	**April 26 – STUDENT RESEARCH PRESENTATION**
16	**May 3** – DUE: **Research (final report) + notebook**	

Guidelines for Formal Reports

Title, Byline and affiliation: The title should clearly state the main objective of the experiment or project. Below the title add your name and the names of those who made substantial contribution to the work and your institution.

Abstract: Provides a summary overview of all parts of the report, usually in a paragraph, often emphasizing the major findings in the study.

Introduction: States the problem and the reason for studying it. Give relevant background of what has been done before problem and what will be addressed by the study. Insert proper reference numbers for citations (see under Citation and References).

Experimental Procedure: Write a detailed procedure for the experiments you preformed (write in the past tense, passive voice and in the third person). Instead of rewriting the procedure given in the lab handout, **write what was actually done. It is important to give sufficient detail so that a person with similar knowledge level as yourself can follow and repeat the experiment.**

Data and Calculations: The first step in completing this section is to use your data and generate any tables or graphs necessary for the analysis. This should be done in your lab notebook. Data may be graphed or tabulated. Whether the results are graphed or tabulated will depend on the data and the conclusions you draw. You need to use your judgment.

Then examine your data and select the appropriate, pertinent items for your formal report. Not everything in the data tables in your notebook will necessarily go into tables in your report. In your notebook you might have recorded initial and final buret readings, but in your report you would only state the volume of titrant used, i.e., the difference between the initial and final buret volumes. Once the reliability of your data has been assessed, you may tabulate your results. Having achieved this, you can discuss and interpret your results.

Conclusions you draw from your data must be presented in a clear, concise manner. Tables and figures (graphs are considered figures) should be integrated into your text, as you would find them in your textbook or in a journal article. You should introduce data tables and figures with words using complete sentences. Refer to figures and tables sequentially as they are introduced. Figures and tables should be identified with a separate series of number

Figures: Figures can be graphs of data, photographs, sketches, flow charts, and so on. Figures can play a major role in highlighting, clarifying, and summarizing data and results and can substantially increase the reader's comprehension of the text by communicating visually. All figures **must** be mentioned or discussed by name and number in the text.

- Capitalize the word "Figure" when it is followed by the figure number.
- Number figures sequentially with arabic numerals in order of discussion in the text (Figure 1, Figure 2, etc.)
- Chemical structures and schemes should not be numbered as figures.
- Every figure **must** have a caption that includes the figure number and a brief, informative description.

Tables: Use tables when data cannot be presented clearly as narrative. Like firures, all tables must be mentioned or discussed by number in text. A table should consist of at least three interrelated columns and three rows.

- Capitalize the word "Table" when it is followed by the table number.
- Number tables sequentially with arabic numerals in order of discussion in the text (Table 1, Table 2, etc.)
- Needs a brief, informative title that describes its content. Begin the table title with the work Table and its number.
- Every column must have a heading

Results and Discussion: This section is the meat of a formal report as it is where you demonstrate your understanding of the experiment and its results. It is also the most difficult to write, should take the most time, and is generally worth the most points in your score.

Begin this section with a statement of results. When you have finished working up your data, look it over to decide what conclusions may be drawn. State your results briefly, using the past tense. Write something about each table or figure, keeping in mind that they present the data but they do not state the results. Do not simply offer the data as your results. Be sure to introduce all your results in this section.

This section will also contain error analysis. Before one can draw conclusions from data, one must assess the precision and accuracy of the results. A result is only as good as the accuracy to which it was measured. To evaluate your data you must know how reliable it is. Acquiring data on a brand-new instrument does not mean that there is no error in the data, nor are computer calculated results error free.

There is always some error in your measurements. In the discussion of each error, a discussion of its effect on the experimental outcome/results should be included. Listed below are some common sources of error, all of which should be considered in assessing your data.

Once you have assessed the reliability of your data, you can discuss and interpret your results. You should first consider whether you accomplished what was proposed in the introduction and if your results were successful. What are the significant sources of error in the experiment? At least three procedural errors should be identified. How might they be minimized in the future?

Begin the "Results and Discussion" section with your interpretation of the results, and then perhaps a comparison of them with expected values. Always try to put a positive spin on your results if possible. You must also discuss the reliability of your data, how the reported uncertainty was determined and what its primary source was.

Discuss and interpret the data and results. This includes (but not limited to) analysis of the spectral data to draw conclusion, identification of the product(s) if unknown, and/or comparison of the characterization data with literature data if the product is known. You may discuss problems you encountered, briefly summarize how the chemical reaction worked and roles of each reagent and condition in the reaction itself as well as the purification process.

Things may go wrong in lab. However, even if your results are questionable, it is still possible to write a good lab report. Begin by stating what should have happened, then discuss what actually happened and why the experiment went wrong. Never begin your discussion with what went wrong. It is important that you demonstrate that you understand both what should have happened and what might have gone wrong. Note also that there is a big difference between a null result and a failure to get results.

Conclusion: The purpose of the Conclusion section is to summarize the pertinent concepts discussed in the R&D section. Always begin your Conclusion by clearly stating your results and the "goodness" or significance of your results, and relating them to ideas presented in the introduction. In other words, if the objective of the study was to determine the percent calcium carbonate in an unknown sample, you should restate the percentage, with its uncertainty, in this Conclusion section.

Important observations may go in this section as well. Discuss the significance of the results. When possible, compare your results with literature values. Discuss significant errors and suggest improvements to the procedure or possible ideas for additional experiments that could further support your conclusion.

Then make a concluding statement(s) and relate your conclusion to the ideas presented in the introduction. Note: Stating that "overall the experiment went well" or that "I learned how to use a piece of equipment" are not strong conclusions.

The conclusion is not to be a lengthy discourse. One paragraph (about four to seven sentences) is the amount to be presented in conclusion

Citation: If you cite or rephrase from literature in any part of your report, you must give **a reference number** after the cited or rephrased sentence and list the references under Reference section (see below). Especially your Introduction will need to show appropriate citations, because most likely the theories and background information discussed are not your original idea! Rephrase and resummarize the citation as much as possible… and NEVER SIMPLY COPY AND PASTE! You are encouraged to change the wordings in the citation to best suited the context. Example:

> A spectrochemical series of ligands is a list of ligands ordered on ligand field-strength exerted on the metal center in metal complexes.[1] In crystal field theory, ligands split the energy levels of the d-orbitals of the metal center (Δ - crystal-field splitting parameter; Δ_{oct} for octahedral crystal field), and the nature of the ligand affects the magnitude of Δ.[2] This energy splitting is reflected in differences in color of metal complexes, where an electron in the lower energy d-orbital is excited to the higher energy d-orbital by absorbing the photon with energy corresponding to Δ.[2]

References: List all relevant literature citations using a proper format (see JACS format below). Must be cited in text, number must be given in the order of appearance in your main text. If you use MS Word, use the Reference function is a convenient one to use (instruction will be given on the first day of class).

Citing References in Text

1. By superscript numbers, which appear outside the punctuation if the citation applies to a whole sentence or clause.

   Fluoridated water as well as various fluoride products such as toothpaste provide fluoride ions necessary for remineralization.[1]

2. The author's name may be made part of the sentence. If a reference has two authors, give both names joined by the word "and". If a reference has more than two authors, give only the first name listed, followed by "et al." Do not use a comma before et al.; always use a period after al.

   Rakita[1] states that fluoridated water as well as various fluoride products such as toothpaste provide fluoride ions necessary for re-mineralization.

3. Start with 1 and number consecutively throughout the paper, including references in text and those in tables, figures, and other non-text components. If a reference is repeated, do not give it a new number; use the original reference number.

4. When citing more than one reference at one place; list the numbers in ascending order and separate them by commas (without spaces), or if they are a part of a consecutive series, use a dash to indicate a range of three or more.

5. Cite the reference in a logical place in the sentence.

Style for Reference list - References always end with a period.

Books

Single author	Chang, R. *General Chemistry: The Essential Concepts*, 3rd ed.; McGraw-Hill: Boston, 2003.
Edited Book	Gbalint-Kurti, G. G. Wavepacket Theory of Photo-dissociation and Reactive Scattering. In *Advances in Chemical Physics;* Rice, S. A., Ed.; Wiley: New York, 2004; Vol. 128; p 257.
Book in Series	*Omega-3 Fatty Acids: Chemistry, Nutrition, and Health Effects;* Shahidi, F., Finley, J. W., Eds.; ACS Symposium Series 788; American Chemical Society: Washington, DC, 2001.
Article from a reference book	Powder Metallurgy. *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed.; Wiley: New York, 1982; Vol. 19, pp 28-62.

Articles

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* **Year**, *Volume*, Inclusive Pagination.

Article in a scientific journal	Evans, D. A.; Fitch, D. M.; Smith, T. E.; Cee, V. J. Application of Complex Aldol Reactions to the Total Synthesis of Phorboxazole B. *J. Am. Chem. Soc.* **2000,** *122*, 10033-10046.
Article in a popular/non-scientific magazine	Manning, R. Super Organics. *Wired*, May 2004, pp 176-181.
Article from an online journal	Peacock-Lopez, E. Exact Solutions of the Quantum Double Square-Well Potential. *Chem. Ed.* [Online] **2007,** *11*, 383-393 http://chemeducator.org/bibs/0011006/11060380lb.htm (accessed Aug 23, 2007).

Web/Online – Note: Different web browsers break the text in different places of a URL. The URL should begin on the same line as the rest of the citation information, with a break inserted after a slash, if needed.

Internet sources include online editions of traditional sources such as periodicals and books. Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* [Online] **Year**, *Volume*, Inclusive Pagination. URL (accessed Month Day, Year)

Electronic copies of periodicals retrieved from subscription database services often provide only the original text but not the original formatting or the figures. Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* [Online] **Year**, *Volume*, Article number or other identifying information. Database provider URL of top page (accessed Month Day, Year)

Web page	National Library of Medicine. Environmental Health and Toxicology: Specialized Information Services. http://sis.nlm.nih.gov/enviro.html (accessed Aug 23, 2004).
Article from an online journal	Peacock-Lopez, E. Exact Solutions of the Quantum Double Square-Well Potential. *Chem. Ed.* [Online] **2007,** *11*, 383-393 http://chemeducator.org/bibs/0011006/11060380lb.htm (accessed Aug 23, 2007).
Article from full text database	Begley, S. When Does Your Brain Stop Making New Neurons? *Newsweek* [Online] July 2, 2007, p 62. Expanded Academic Index. http:/galegroup.com (accessed Aug 23, 2007).

* Note that web pages may disappear anytime and many of they are not considered appropriate sources.

*Wikipedia is a useful site to get basic information, but it is not suitable to cite in an academic writing.

* First check if it is an online version of a published article. If it is, follow the journal article citation format (see above). Otherwise, after making sure that the qualification of the author of the website and the quality/validity of the site, use the following examples as a guideline.