Chem 4352/8352
Physical Organic Chemistry
Spring Semester, 2017
MWF 10:10-11:00 a.m. Rm 121 Smith Hall

Instructor: Steven Kass, 223 Smith Hall, 625-7513 (kass@umn.edu)

Text: "Mechanism and Theory in Organic Chemistry", by Thomas H. Lowry and Kathleen Schueller Richardson, 3rd Edition, Harper and Row: New York, 1987. Additional reading material will be noted and made available through out the semester.

Office Hours: Steven Kass: M 4:00 - 5:00 p.m., W 11:00 a.m. - 12:00 p.m. or by appointment.

Exams: There will be two 2 hour midterm exams.

Midterm I: Wednesday, March 8
Midterm II: Wednesday, April 26

Problem Sets: Five problem sets with given due dates will be assigned during the course of the semester. These are to be done individually, but you are free to discuss them with your classmates.

Paper/Project/Presentation:

Graduate students will work in groups of 2 or 3 and write a 4-6 page paper on a physical organic chemistry topic addressing a mechanism, reactive intermediate, chemical interaction or spectroscopic technique. The emphasis should be on experimental results and not computations. Papers are required to be double-spaced in 12 pt font with 1" margins and references in *JACS* style format. Topics must differ from material covered in class, be preapproved by the instructor, and will be available on a first come first serve basis; each group will work on different topics. Papers are due in class on Monday, April 24 and 10-15 minute presentations will take place the last week of classes. The aim is to teach the class about a subject not covered in lecture. Possible topics include: (1) molecular recognition, (2) halogen bonding, (3) counterion catalysis, (4) endohedral fullerenes or carceplexes, (5) molecular motors, (6) methylene (CH_2:), (7) Marcus theory, (8) isothermal calorimetry, (9) cyclohexyne, (10) carbyne, (11) SOMO catalysis, (12) proton coupled electron transfer.

Grading: The final grades will be determined based upon the results of the 2 exams and the problem sets as follows:

Chem 8352 students: Problem Sets = 6% each (total = 30%)
Midterm Exams = 25% each (total = 50%)
Written/Oral Project 20%

Chem 5352 students: Problem Sets = 10% each (total = 50%)
Midterm Exams = 25% each (total = 50%)

Subjects: An approximate listing and sequence of the topics to be covered.

Thermochemistry and symmetry
Hybridization and bonding
Small ring chemistry
Hückel Theory
Aromaticity/Antiaromaticity
Frontier Molecular Orbital Theory
(Semi-empirical calculations)
Woodward Hoffmann Rules/Pericyclic Reactions
Modern techniques for studying reactive intermediates
(Gas Phase Ion-Molecule Chemistry, Laser Flash Photolysis, Photoacoustic Calorimetry
Free Radicals and ESR spectroscopy
Photochemistry
Miscellaneous problems covering carbanions, cations, carbenes, etc. also will be covered through out the semester.

Reading Materials:

1. Handouts and articles.
2. "The Conservation of Orbital Symmetry", by R. B. Woodward and R.Hoffmann, Academic Press: 1971.
3. "Thermochemical Kinetics", by S. Benson, John Wiley: New York, 1976.
4. "Chemical Applications of Group Theory", by F. A. Cotton, John Wiley: New York, 1971.
5. "Determination of Organic Reaction Mechanisms", by B. Carpenter, John Wiley: New York, 1984.
6. "Advanced Organic Chemistry: Reactions, Mechanisms, and Structure", 3rd Ed., by J. March, McGraw-Hill: New York, 1985.
7. "Quantum Mechanics for Organic Chemists", by H. E. Zimmerman, Academic Press: New York, 1975.
8. "Orbital Symmetry: A Problem Solving Approach", by Roland E. Lehr and Alan P. Marchand, Academic Press: New York, 1972.
9. "Frontier Orbitals and Organic Chemical Reactions", by Ian Fleming, John Wiley: New York, 1976.
10. "Molecular Orbital Theory for Organic Chemists", by A. Streitwieser, John Wiley: New York, 1961.
11. "Modern Molecular Orbital Theory for Organic Chemists", by Weston T. Borden, Prentice Hall: New Jersey, 1975.

Student Academic Integrity and Scholastic Dishonesty

Academic integrity is essential to a positive teaching and learning environment. All students enrolled in University courses are expected to complete coursework responsibilities with fairness and honesty. Failure to do so by seeking unfair advantage over others or misrepresenting someone else's work as your own, can result in disciplinary action. The University Student Conduct Code defines scholastic dishonesty as follows:

Scholastic Dishonesty: Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering forging , or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis. Within this course, a student responsible for scholastic dishonesty can be assigned a penalty up to and including an "F" or "N" for the course. If you have any questions regarding the expectations for a specific assignment or exam, ask.

How to Avoid Plagiarism

Author: Anonymous. Edited by Phil Buhlmann

From Dr. Phil Buhlmann and his class Analytical Spectroscopy, I have learned a lot more than just Chemistry. Maybe you have a much clearer idea about what I am going to write below. Anyway, I still hope that what I explain will be somewhat helpful to you.

When reading *Analytical Spectroscopy*'s syllabus, I felt a little weird when reading the part about plagiarism because I never saw any teacher include anything like that in a syllabus. I even thought it was a little strange and had nothing to do with me. At last, I found out it was not strange at all. It is really serious! When finishing my final report for this class, I made a serious mistake; not a small mistake but a huge mistake! In this report, we were required to review three analytical techniques that we discussed earlier in class. I copied a lot of paragraphs from the original articles and from a web site directly into my report. On a web site, I found some information on the background of the problem. From the original articles, I copied the abstracts to give a general idea about the individual methods of analysis. The big problem is that I copied and pasted most of the information for my final report, actually more than two thirds. Even though I made a little summary at the end of the report, it did not change the fact that most of the report did not reflect my own ideas. What I did was just organize them, bring them together, in other words collect them. I know now most of you would say that "You were cheating". Yes, now I know I was totally wrong. However, when I wrote this report, I did not realize it would be plagiarism. If I had known, I would not have done it!

When copying the background information from the web site, I knew my review should not be longer than 3000 words. How could I think of so many words? I copied and pasted a lot of sentences and paragraphs directly from the articles. At the time I did it, I thought it was acceptable for a review. I thought it was only my job to introduce information. When introducing these methods, I did not think that I could think of a better way to formulate it than the original authors. So I took the original authors' sentences as the introduction and I thought it would be acceptable if I just cited references.

I am not looking for excuses for my mistakes, believe me. Now after a long and useful discussion with Dr. Buhlmann, I understand that the most important issue was not to formulate the content of my review without any grammatical errors, but expressing my ideas in a scientific way on my own. I have now another understanding of what a review is. I thought that since I didn't do any new experiments by myself, I could not contribute any new information myself,

and all I could do was to report to readers other persons' ideas. I was wrong. I can add my ideas into a review. For example, I can point out aspects that were not mentioned in the original papers paper. I can point out assumptions that were not mentioned. Also, I can critically compare methods discussed by different authors, where the authors of the original articles did not attempt any comparison of one's another work.

Another fault of mine was in the way I was giving references. Even though I listed at the end of the report the web site and articles from which I had copy-pasted whole paragraphs, I did not make it clear to readers that I had actually copy-pasted whole paragraphs. For example, I copied two paragraphs from one article and I gave a reference to that article at the end of the first paragraph. However, by only giving the reference, I know now I implied that the reference gave information relevant to my paragraph. However, I realize now that it was not obvious to my readers that I had copy-pasted two whole paragraphs. To emphasize that a whole paragraph is copy-pasted, I should have marked it more clearly. For example, I could have indented the whole paragraph, set the whole paragraph in italics, or set the whole paragraph in quotation marks.

Dr. Buhlmann introduced me to a good book *The Chicago Manual of Style*. This book talks a lot about how to give clear references. Below are some guidelines that I found in this book:

1. The most common way to give a [verbatim] reference is to give it in the text with parentheses. Part of or the whole sentence or paragraph should be enclosed in parentheses.1
2. If frequent citations from one source are used, each needs reference location. The preferred way is to give a locating page, line number, and part in parentheses following each citation.1

With the prevalence of the internet, it is easy to find a lot of relevant information about almost any topic. However, we have to know that information that we find on web sites has the same copyright problem as hard copy books. (This paragraph is paraphrased from the web site *http://www.plagiarism.org/plagiarism.html*). 2

References

1. *The Chicago Manual of Style,* 14th edition, Page 379-381, the University of Chicago Press
2. *http://www.plagiarism.org/plagiarism.html*