

CHE 175: MECHANISTIC ORGANIC CHEMISTRY III

Spring, 2002

Dr. Matthew R. Dintzner

O'Connell 440, 446 (Lincoln Park Campus)

(773) 325-4726, office (773) 325-4725, lab

<http://www.depaul.edu/~mdintzne>

Office Hours: Mondays 3:00-5:00 p.m., Tuesdays 9:30-11:30 a.m., or by appointment.

Course Description and General Objectives: This is the third in a sequence of courses designed to investigate what organic chemistry is and how it works, by emphasizing the relationship between structure and function of organic molecules. In this course we will build on the foundation established in the first two quarters, which was based on unifying principles of reactivity (electrophilic additions, radical substitutions, nucleophilic substitutions, eliminations, electrophilic aromatic substitutions, nucleophilic acyl substitutions, and nucleophilic additions). At this stage, you are expected to be familiar (if not proficient) with the following topics as they relate to organic chemistry: atomic and molecular structure and how to represent them using the Lewis dot convention, hybridization, bonding, physical properties, nomenclature (IUPAC and common) of organic molecules, polarity (dipole moments), principles of thermodynamics and kinetics, stereochemistry, electron delocalization and resonance, spectrometry and spectroscopy (MS, IR, NMR), and aromaticity. You should understand the difference between a nucleophile and an electrophile, how to identify the nucleophilic and electrophilic components of any given reaction. You should understand what an organic reaction mechanism is and the convention for writing one (arrow-pushing). You should understand regiochemical and stereochemical consequences of reactions. All of the fundamental skills that you have developed during the first two quarters of this course-sequence will be applied to the organic chemistry of living systems this quarter.

Texts: *Organic Chemistry (3rd ed.)* by Paula Yurkanis Bruice, with *Study Guide and Solutions Manual*.

Quizzes: Quizzes will be given during the first 30 minutes (or so) of quiz section on Tuesdays throughout the quarter; the remainder of the quiz section will be used for pre-lab lecture. The two lowest quiz-grades will be dropped. The format for quizzes will be: 4 short-answer questions or problems (40 %, or 10 pts each) and 10 multiple choice questions (60 %, or 6 pts each).

Final Exam: The ACS standardized exam (70 multiple-choice questions) will be administered on Thursday, June 13, 2002 (11:45 a.m. – 2:00 p.m.) as the final exam for the course sequence. It is cumulative for all three quarters and will count for 25 % of your overall grade.

Grades: Final grades will be based on the scale and distribution shown below. If the overall class average is NOT between 77 and 82, final grades will be curved accordingly so that the average grade is B-/C+.

93 – 100, A	83 – 86, B	73 – 76, C	60 – 66, D
90 – 92, A-	80 – 82, B-	70 – 72, C-	< 60, F
87 – 89, B+	77 – 79, C+	67 – 69, D+	

Quizzes = 50 %

Final Exam (ACS Exam) = 25 %

Lab = 25 %

Schedule: The following is an outline of the material we will cover throughout the quarter. This schedule is subject to change as a function of class-performance and understanding of the individual topics (we will spend additional time on some topics if necessary). The reading assignments are from your text (Bruice).

DATE	READING ASSIGNMENT (please read ahead)	SPECIFIC TOPICS AND LABS	✓
M 4/1	17.1-17.3	Aldehydes and ketones: nomenclature, relative reactivities.	✓
T 4/2	17.4-17.6	Reactions of carbonyl compounds with carbon nucleophiles, Grignard reagents and hydride ion.	✓
W 4/3	17.7	Reactions of carbonyl compounds with nitrogen nucleophiles.	✓
F 4/5	17.8-17.10	Reactions of carbonyl compounds with oxygen and sulfur nucleophiles; protecting groups.	✓
M 4/8	17.11-17.16	Wittig reaction; stereochemistry of addition reactions to carbonyls; intramolecular reactions; addition of nucleophiles to α,β -unsaturated carbonyls (direct vs. conjugate).	✓
LAB 1	Handout	Synthesis of the Insect Repellent DEET	✓
T 4/9	QUIZ	1	✓
W 4/10	18.1	Reduction reactions.	✓
F 4/12	18.2-18.5	Oxidation reactions.	✓
M 4/15	18.6-18.11	Oxidative cleavage reactions; synthetic considerations;	✓

		biological oxidation-reduction reactions; quinones.	
LAB 2	G/M 20.1 20.2 A-E miniscale	Synthesis of Sulfanilamide (start)	✓
T 4/16	QUIZ	2	✓
W 4/17	19.1-19.3	Reactions at the α -carbon of carbonyl compounds; keto-enol tautomerism.	✓
F 4/19	19.4-19.9	Halogenation at the α -carbon; using LDA to generate an enolate; alkylation at the α -carbon; enamines	
M 4/22	19.10-19.13	The Michael reaction; aldol addition and condensation reactions; mixed aldol reactions.	
LAB 3	20.2 A-E miniscale	Synthesis of Sulfanilamide, continued (finish)	
T 4/23	QUIZ	3	
W 4/24	19.14-19.20	Claisen and mixed Claisen condensations; intramolecular condensation reactions; decarboxylation; malonic ester and acetoacetic ester syntheses.	
F 4/26	20.1-20.5	Carbohydrates: classification, configuration, redox reactions.	
M 4/29	20.6-20.10	More carbohydrate reactions.	
LAB 4	G/M 18.3 microscale	Synthesis of <i>trans</i> -p-Anisalacetophenone	
T 4/30	QUIZ	4	
W 5/1	20.11-20.21	Monosaccharides, glucosides, disaccharides and polysaccharides, carbohydrate-derived natural products.	
F 5/3	21.1-21.4	Amino acids: classification, configuration, physical properties.	
M 5/6	21.11-21.15	Proteins: primary, secondary, tertiary, quaternary structures.	
LAB 5	Handout	Hydrolysis of Polysaccharides	
T 5/7	QUIZ	5	
W 5/8	22.1-22.5	Catalysts and catalysis in organic reactions.	
F 5/10	22.8-22.10	Catalysts in biological reactions: enzymes and antibodies.	
M 5/13	23.1	Metabolism: overview.	
LAB 6	Handout	Isolation of Fats, Proteins and carbohydrates from Milk	
T 5/14	QUIZ	6	
W 5/15	24.1-24.3	Lipids: fatty acids, waxes, fats and oils.	
F 5/17	24.4-24.6	Membranes, prostaglandins and terpenes.	
M 5/20	24.7-24.11	Vitamin A, terpene biosynthesis, steroids.	

LAB 7	Handout	The Fatty Acid Composition of Fats	
T 5/21	QUIZ	7	
W 5/22	25.1-25.4	Nucleosides and nucleotides, ATP, phosphoryl transfer reactions.	
F 5/24	25.5-25.14	Nucleic acids, DNA, RNA.	
M 5/27	NO	CLASS	
LAB 8	Handout	Synthesis of Luminol	
T 5/28	QUIZ	8	
W 5/29	29.1-29.2	Multistep organic synthesis, retrosynthesis.	
F 5/31	29.3-29.4	Retrosynthesis cont'd, protecting group manipulation.	
M 6/3	29.5-29.6	Stereochemistry in synthesis.	
T 6/4	QUIZ	9	
W 6/5	REVIEW	Focus on material from CHE 171; <i>come with questions</i>	
F 6/7	REVIEW	Focus on material from CHE 173; <i>come with questions</i>	
Th 6/13	FINAL EXAM	11:45-2:00 p.m.	

LAB:

Objectives: In addition to good laboratory techniques and the methods of carrying out basic laboratory procedures, other things you will also learn from this laboratory course are: (1) how to take data carefully; (2) how to record relevant observations; (3) how to use your time effectively; (4) how to assess the efficiency of your experimental method; (5) how to plan for the isolation and purification of the substance you prepare; (6) how to work safely; (7) how to solve problems and think like a chemist.

Lab Text: *Experimental Organic Chemistry*, by Gilbert and Martin (Saunders College Publishing) and additional handouts.

Teaching Assistants: Kristen McColough (Tuesday), Debbie Coligado (Thursday).

General Rules:

- Safety goggles are to be worn at all times when in the laboratory; wear gloves when necessary.
- No shorts, sandals or rollerblades are to be worn in the laboratory.
- Please read and be familiar with the University's Chemical Hygiene Plan.
- Please respect the laboratory space and your classmates by cleaning up after yourself.
- Please come to lab prepared by reading over the experiment prior to your laboratory period.

***** Prepare your notebook AHEAD OF TIME. You will NOT be allowed to bring your textbook into the lab, so you'll rely solely on your notebook to get you through the experiment. Be sure that you can read your notes and that they make sense to you.*****

Lab Grades: Your notebook is your "ticket" into the lab, and will be checked by your T.A. as you enter. This is not meant to be a scare tactic-- you'll find that the better prepared you are for lab, the quicker you'll finish the experiment and the better will be your results... it just makes sense. Your T.A. will also be responsible for grading your lab reports and observing your lab technique. The overall lab grade is based on the following distribution:

Lab Reports	75%
Notebook	20%
Technique	5%

Notebooks: Prepare your notebook AHEAD OF TIME according to the guidelines below. You will NOT be allowed to bring your textbook into the lab, so you'll rely solely on your notebook to get you through the experiment.

Key Components of a Laboratory Experiment Notebook:

(1) Date experiment was conducted; (2) Title of experiment and reference for it; (3) Purpose for running the reaction; (4) Reaction scheme, a balanced equation (if applicable); (5) Table of reagents and product with data on the compounds' names, physical constants like MF, mp, bp (literature and experimental values), density, volume, weight and moles, theoretical and percent yield (where applicable), safety information related to exposure and toxicity from the Material Safety Data Sheets (MSDS); (6) Details of procedure and set-up used and all changes from procedure from the lab manual; (7) Characteristics of the products; (8) Analytical and spectral data.

Always record your data in ink. If a mistake is made, make a neat line through the word or words so they remain legible. Write and organize your work so that someone else could come into the laboratory and repeat the experiment using your directions without confusion and uncertainty. Completeness and legibility are key factors. Make sure your notebook is signed by the TA at the end of each lab period. (This does not mean that the TA has approved your method of taking data).

Lab Reports: The purpose of the laboratory report is to give a complete and concise description of the experiment. All lab reports must be turned in to your TA one week after the experiment is completed. Turning in lab reports after the due date will result in a loss of 10 points, minus 5 points for each day after the due date. No lab reports will be accepted after March 18th. Formal laboratory reports should be typed (no more than 3-5 pages, double-spaced with figures, illustrations, etc.) according to the guidelines below.

Lab Report Format:

(The headings printed in bold-face below should appear in your lab report)

- Lab #_____ Date of Experiment:
- Experiment # and Title (from textbook), Date of Report:
- References: (lab manual, handbooks, etc.)
- Purpose: One or two sentences telling the objective of the experiment.
Failure to include the above information can lose you 5 points.
- Equation and reactions: (5 points) Write a balanced equation, if the experiment involves a synthesis.
- Procedure: (10 points) You may reference your lab textbook and note only those reagents, steps, and equipment that have been changed.
- Results: (25 points) Data include all observations and numbers as transcribed from your lab notebook. The should be neatly written in tabular form when appropriate. Units must be shown. The calculation for the limiting reagent (when appropriate) and the theoretical yield should be included.
- Discussion: (30 points) Discuss your data and observations as they relate to the reactions and the experiment in a logical manner. You must talk about your results in a way that describes how your results support your lab objective. Exclude those points that are not relevant to your experiment.
- Conclusion: (10 points) This section sums up the lab. It re-tells your lab's objectives and says how the results helped you to achieve these objectives or not. This section does not simply say if your lab was a success or not. We will be the judges of that.
- Answers to Questions at the end of the experiment; check with your TA (15 points).

General Guidelines for the Organic Chemistry Laboratory:

- Study the experiment and the reasons for each operation before you come to lab. Study, do not just read about the experiment before lab period. Although the techniques employed in the laboratory are not particularly difficult to acquire, they do demand a significant amount of attention. For you to reach a successful and happy conclusion, you cannot afford to have the focus of your concentration broken by having to constantly refer to the text during the experiment (this is why the texts are not allowed in the lab). Disaster is ever present for the unprepared.
- ALWAYS work with clean equipment. You must take time to scrupulously clean your equipment before you start any experiment. Contaminated glassware will ultimately cost you additional time, and you will face the frustrations of experiencing inconsistent results and lower yields.
- CAFEFULLY measure the quantities of materials to be used in the experiments. A little extra time at the beginning of the laboratory can speed you on your way at the end of the session.

Many organic reactions are very sensitive to relative quantities of reagents. Do not be hurried or careless at the balance.

- *Clean means DRY. Water or cleaning solution can be as detrimental to the success of a reaction as dirt or sludge in the system.
- ALWAYS work on a clean laboratory bench surface.
- ALWAYS place reaction vials or flasks in a clean beaker when standing them on the laboratory bench.
- ALWAYS think through the next step you are going to perform before starting it. Once you have added the wrong reagent, it is back to square one.
- ALWAYS save everything you have generated in an experiment until it is successfully completed. You can retrieve a mislabeled chromatographic fraction from your locker but not from the waste container.
- ALWAYS keep a permanent record of all lab work in a bound notebook.

ACADEMIC DISHONESTY:

ANY VIOLATION OF THE ACADEMIC HONESTY POLICY IN THE CLASSROOM, DURING QUIZ SECTION, OR IN THE LABORATORY IS EXTREMELY SERIOUS. READ THE APPROPRIATE SECTIONS OF THE STUDENT HANDBOOK FOR THE POLICY.