CHEMISTRY 331 - Spring 2010
Environmental Organic Chemistry

This course will examine mechanisms of organic transformations and the fate of molecules of environmental significance. Topics include partitioning, hydrolysis, oxidation-reduction and photolysis. The laboratory emphasizes techniques used in physical organic chemistry, including, kinetics, thermodynamics, linear free energy relationships and adsorption phenomena.

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Textbook:
Environmental Organic Chemistry, 2nd Ed., R.P. Schwarzenbach, P.M. Gschwend, D.M. Imboden, J Wiley, 2002.

Supplementary Materials (on Course Reserve in Library) :
Structure and Reactivity in Organic Chemistry, H. Maskill, Oxford University Press, 1999.
Mechanisms of Organic Reactions, H. Maskill, Oxford University Press, 1996.
Reaction Mechanisms in Environmental Organic Chemistry, R.A. Larson, E.J. Weber, Lewis, 1994.
Theory and Mechanism in Organic Chemistry, T.H. Lowry; K.S. Richardson, J Wiley, 1987.
Illustrated Handbook of Physical-Chemical Properties And Environmental Fate For Organic Chemicals, Volumes 1 – 5, D. Mackay; W.Y. Shiu; K. C. Ma, Lewis Publishers, 1992.

Prerequisites: CHEM 232 **Recommended:** CHEM 221

Course Delivery:

Lectures	**M W** 1:00 - 2:20	B200, Rm 106
Labs	**W** 2:30 - 6:20	B360, Rm 201 (alternate weeks starting Jan. 13th)
Tutorials*	**F** 11:30-12:20	B200, Rm106 (one hour per week)

Course Evaluation:

Final Exam	40%	(three hour final)
Lab	20%	(four formal lab reports @ 5% each)
Mid-Terms	15%	(tentatively February 15th & March 15th)
Research Poster	15%	(March 22nd)
Assignments	10%	(four assignments @ 2.5% each)

** Tutorials are scheduled each Friday to cover review materials, address assignment and laboratory questions. Attendance is mandatory.*

CHEM 331 - COURSE OUTLINE
ENVIRONMENTAL ORGANIC CHEMISTRY

1. INTRODUCTION AND REVIEW (Chapters 1 and 2)
Classification of organic molecules and review of physical properties including, natural organic matter, halocarbons, phenols, polyaromatic hydrocarbons, organophosphates, surfactants; Review of sources such as agrochemicals, industrial uses, flame retardants and by-products.

2. CHEMICAL DISTRIBUTION IN THE ENVIRONMENT (Chapters 3 – 11 and handouts)
Introduction to the molecular interactions that lead to physical properties that affect chemical distribution in the environment.

2.1 MOLECULAR PARTITIONING (selections from Chapter 3)
Molecular interactions; partition constants; thermodynamic considerations

2.2 VAPOUR PRESSURE (Chapter 4)
Thermodynamic considerations; molecular interactions; temperature; estimation methods

2.3 WATER SOLUBILITY (Chapter 5)
Thermodynamic considerations; activity coefficients; excess free energy; effect of temperature and ionic strength; estimation methods; molecular fragment contributions

2.3 AIR- WATER PARTITIONING (Chapter 6)
Thermodynamic considerations; Henry's Law constant; estimation methods

2.4 OCTANOL – WATER PARTITIONING (Chapter 7)
Thermodynamic considerations; linear free energy relationships; estimation methods

2.5 ACID – BASE PARTITIONING (selections from Chapter 8)
Acidity constants; substituent effects; Hammett equation; effect of water solubility

2.6 SORPTION PARTITIONING (selections from Chapters 9 – 11)
Solid – water (K_d) interfaces; sorption to particulate and dissolved organic matter; bioaccumulation; biomagnification; sorption to inorganic surfaces

3. CHEMICAL TRANSFORMATIONS IN THE ENVIRONMENT (Chapters 12 - 16)
Introduction to important reaction classes of organic molecules including substituent effects and structure – activity relationships.

3.1 NUCLEOPHILIC REACTIONS: HYDROLYSIS (Chapter 13)
Functional group transformations including reactions with epoxides, halocarbons, phosphate esters and carboxylic acid derivatives; Mechanisms of hydrolysis reactions; Kinetics, substituent effects and linear free energy relationships (Hammett)

3.2 REDUCTION REACTIONS (Chapter 14)
Mechanisms of reductive transformation pathways including dehalogenation and nitroaromatic reductions; Introduction to electron mediated reductions involving NOM

3.3 OXIDATION REACTIONS (Chapter 14)
Oxidations involving molecular oxygen, superoxide, singlet oxygen and ozone; Oxidations involving hydroxyl radicals and by-products; Reactions with disinfectants, aqueous chlorine

4. SPECIAL TOPICS: (selected readings and guest lectures)
March 24th, Dr. Trisha Huber, Defence Scientist, CFB Esquimalt - Properties and Applications of Carbon Nanotubes
March 31st, Dr. Rob Macdonald, Research Scientist, IOS - Fate and Distribution of Persistent Organic Pollutants
April 7th, Tim MacInnis, AERL/UVic graduate student - Environmental Photochemistry

TBA - Remediation strategies incineration, bioremediation, advanced oxidation and electroreduction.

CHEM 331 LABORATORY

January 13th **The Octanol-Water Partition Co-efficient**
Using HPLC retention times to estimate the K_{ow}.

January 27th **Stir Bar Solvent Extraction Analysis of PAHs in Aqueous Solution**
Using a polymer based technique to pre-concentrate polyaromatic hydrocarbons for analysis by GC-MS.

February 10th **Linear Free Energy: The Hammett Equation**
Evaluating the pKa's of substituted benzoic acid derivatives by acid-base titration.

March 3rd & March 17th **Hydrolysis Kinetics of a Carboxylic Acid Ester**
Following the rate of reaction for 4-nitrophenyl acetate under neutral and basic conditions using UV-vis absorption.

March 31st **Photocatalytic Destruction of an Organic Dye Using Titanium Dioxide**
Following the photodegradation of Malachite green using UV-vis absorption.

FORMAL LAB REPORTS

Theory: This section will typically be 2 – 3 pages and will introduce the basic concepts of the lab exercise. Some of this background is given in the lab manual, which you may incorporate in your own words. The theory section will typically involve references from one of more of the course texts.

Experimental: Refer to the lab manual except where modifications have been made. Also include specific information about the source (and purity) of chemical reagents used, make and model of specific instruments employed and operating conditions for instrumental methods. Be sure to describe how duties and responsibilities were divided for labs that involved a group effort.

Data: Summarize experimental data in tables wherever possible. Include enough information for the data table to stand alone as a source of information. Be sure to report the source of data if not your own.

Results: Summarize results in tables where possible. Be sure to include sample calculations (if any) and attach spreadsheet calculations and graphs as an appendix.

Discussion: Discuss the significance of your results in the context of the theory section. Your discussion should include references to the primary literature so that you can compare your results to those of others. Address any supplemental questions in your discussion section. The discussion section will typically be 2- 3 pages.

Each lab report will be marked out of **25** and will be evaluated on organization and presentation as well as content. Be sure to cite all references properly using the ACS style of the journal *Environmental Science and Technology*.

ADDITIONAL RESOURCES

BOOKS

Physical Organic Chemistry

Theory and Mechanism in Organic Chemistry, T.H. Lowry; K.S. Richardson, J Wiley, 1987.
Advanced Organic Chemistry; Part A: Structure and Mechanisms, F.A. Carey; R.J. Sundberg, Plenum, 1986.
The Physical Basis of Organic Chemistry, H. Maskill, University Press, 1985
A Guidebook to Mechanisms in Organic Chemistry, P. Sykes, Longman Publishers, 1986.

Environmental Chemistry

Environmental Chemistry: A Global Perspective, G.W. vanLoon; S.J. Duffy, Oxford Univ. Press, 2000.
Environmental Chemistry, N. Bunce. Wuerz Publishers, 1994.
Environmental Chemistry 6th edition, S.E. Manahan, Lewis Publishers, 1994.
Chemistry of the Environment, T.G. Spiro; W.M. Stigliani, 2003.
Environmental Chemodynamics: Movement of Chemicals in Air, Water, and Soil, L.J. Thibodeaux, J. Wiley, 1996.
Partition and Adsorption of Organic Contaminants in Environmental Systems, C.T. Chiou, J. Wiley, 2002.

Aquatic Chemistry

Organic Chemicals in the Aquatic Environment. Distribution, Persistence and Toxicity, A.H. Neilson, Lewis Publishers, 1994.
Water Chemistry, M. Benjamin, McGraw-Hill, 2002.
Principles and Applications of Aquatic Chemistry, F.M.M. Morel; J.A. Hering, Wiley-Interscience Publishers, 1993.

Handbooks

Illustrated Handbook of Physical-Chemical Properties And Environmental Fate For Organic Chemicals, D. Mackay; W.Y. Shiu; K. C. Ma, Lewis Publishers, 1992.
Handbook of Property Estimation Methods for Environmental Chemicals: Environmental and Health Sciences, R.S. Boethling; D. Mackay, Lewis Publishers, 2000.
Handbook of Groundwater Contaminants, Lewis Publishers, 1994.

Pesticides

Chemistry of Pesticides, K.H. Büchel, J. Wiley, 1983.
Fate and Prediction of Environmental Chemicals in Soils, Plants, and Aquatic Systems, M. Mansour, Lewis Publishers, 1993.

Photochemistry

Aspects of Organic Photochemistry, W.M. Horspool, Academic Press, 1976.
Photochemistry of Environmental Aquatic Systems, R.G. Zika, W.J. Cooper, American Chemical Society Press, 1987.

PERIODICALS

Environmental Science and Technology (American Chemical Society)
Journal of Chemical Education (American Chemical Society)
Journal of Environmental Chemistry (CSIRO Publishing)
Journal of Photochemistry and Photobiology A: Chemistry (Elsevier Publishing)
Chemosphere (Elsevier Publishing)