

#### Republic of the Philippines OFFICE OF THE PRESIDENT COMMISSION ON HIGHER EDUCATION

#### CHED MEMORANDUM ORDER (CMO) No. <u>18</u> Series 2007

## SUBJECT: POLICIES AND STANDARDS FOR BACHELOR OF SCIENCE IN CHEMISTRY (BS CHEM)

In accordance with the pertinent provisions of Republic Act (RA) No. 7722, otherwise known as the "Higher Education Act of 1994," and for the purpose of rationalizing the chemistry education in the country with the end view of keeping apace with the demands of global competitiveness, the following Policies and Standards are hereby adopted and promulgated by the Commission.

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# ARTICLE I INTRODUCTION

#### Section 1 Background

Chemistry is the branch of the natural sciences that study matter, its composition, properties and reactions. It is a broad field, which overlaps with other fields particularly biology, physics and geology. Chemistry also has a role of interconnecting other fields and has thus been described as the Central Science.

The core disciplines of chemistry are inorganic, organic, analytical, physical chemistry and biochemistry.

Chemistry is beneficial to society. It is the foundation science for many industrial and agricultural processes that produce useful products that contribute to the improvement of the quality of life. It is a science of numerous opportunities.

Chemistry is essential for the continued development of the Philippines. Therefore, any policy designed to upgrade chemistry education at the college level should take into account the diversity of chemistry, the need for more trained personnel and the significant investment needed to sustain an acceptable standard of chemistry education.

## Section 2 Objectives of these Policies and Standards

The objectives of the Policies and Standards are as follows:

- a. To set a minimum level of quality for the BS Chemistry program. The main components are: curriculum and course content, faculty, equipment and facilities, and library.
- b. To enable institutions to produce chemists who can practice the profession under the current global standards

# ARTICLE II AUTHORITY TO OPERATE

#### Section 3

All private higher education institutions (PHEIs) intending to offer the Bachelor of Science in Chemistry must secure proper authority from the Commission in accordance with existing rules and regulations. State universities and colleges (SUCs), and local colleges and universities should likewise strictly adhere to the provisions in this policies and standards.

# ARTICLE III PROGRAM SPECIFICATIONS

## Section 4 Degree Name

The degree program herein shall be called Bachelor of Science in Chemistry (BS Chem).

# Section 5 Program Description

## 5.1 Nature of the program

The BS Chem program is a unique program designed for students interested in the science of chemistry and the practice of its profession.

# 5.2 Objectives of the program

- a. Produce graduates who comply with the current qualification requirements for professional chemists for local and overseas employment; and
- b. Prepare students for higher studies in chemistry and in other fields.

# 5.3 Specific professions/careers/occupations or trades that a BS Chemistry graduate may go into.

With a BS degree and professional license, a graduate can be employed at entry-level positions as analytical or laboratory chemist in private industries and companies that deal with pharmaceuticals, food and beverage, cosmetics, oil and petroleum, mineral and metals, environmental analysis, textile, quality control, chemical manufacture, agricultural products research, hospitals, pulp and paper, among others. Graduates can also be employed in government agencies with similar lines of concern and in crime laboratories for forensic analysis.

The BS Chemistry degree holder can also secure non-laboratory work such as science communication, technical writing, marketing and management, product sales, chemical information services, health and safety, patents, project management, etc.

A BS graduate can also be employed as teaching assistants in colleges and universities. Further training (MS and PhD) would qualify graduates for tenured positions in the academe. Passing the local Licensure Exams for Teachers (LET) would qualify graduates to teach in high schools.

## Section 6 Allied Fields

These following fields are recognized to have specializations in chemistry and their graduates may be considered to teach non board courses in the BS Chemistry program such as: marine science, geological sciences, physics, molecular biology and biotechnology, materials science, pharmaceutical science, food science, agricultural sciences, chemical engineering, forensic sciences and environmental science.

# ARTICLE IV COMPETENCY STANDARDS

## Section 7 Core Competencies

The graduate of the BS Chemistry program is expected to possess a wide range of abilities and skills identified in the Euro bachelor<sup>1</sup> program. These are divided into three broad categories:

<sup>&</sup>lt;sup>1</sup> 2003 Chemistry Eurobachelor program (www.cpefr.fr/ectn/tuning%20eurobachelor.htm)

- a. Chemistry-related cognitive abilities and skills, i.e. abilities and skills relating to intellectual tasks, including analysis of problems and systematic problem-solving;
- b. Chemistry-related practical skills, e.g. skills relating to the conduct of laboratory work, proper use of sophisticated instrumentation, safe handling of chemicals and waste minimization; and
- c. Generic skills that may be developed during the course and which are applicable in many other contexts.

The specific skills under each category are:

# 7.1 Chemistry-related cognitive abilities and skills

- a. Conceptual understanding and problem solving skills in the fundamental chemical sub-fields of analytical, organic, inorganic, biochemistry and physical chemistry.
- b. A foundation of physics and mathematics and ability to apply them to chemical problems.
- c. Skills in the evaluation, interpretation and synthesis of chemical information and data, and to draw conclusions from them; ability to assess primary papers critically
- d. Ability to recognise and implement accurate and precise scientific measurements
- e. Computational and data processing skills, relating to chemical information and data.

# 7.2 Chemistry-related practical skills

- a. Skills required in good laboratory practices including safety, waste management and record keeping.
- b. Proper use of modern chemical instrumentation as suggested in section 22.3b (page 56).
- c. Skills required for the conduct of standard laboratory procedures involved and use of instrumentation in analytical and synthetic work, in relation to both organic and inorganic systems
- d. Skills in the monitoring, by observation and measurement, of chemical properties, events or changes, and the systematic and reliable recording and documentation thereof
- e. Ability to evaluate and interpret data derived from laboratory observations and measurements in terms of their significance, and to relate them to appropriate theories
- f. Ability to design experiments and understand the limitations of the experimental approach; ability to design suitable alternative procedures and methods

## 7.3 Generic skills

- a. Communication skills, covering both written and oral communication. This includes the ability to present scientific information in a clear and concise manner and to discuss them intelligently, both in writing and orally.
- b. Ability to dissect a problem into its key features; Problem-solving skills, relating to qualitative and quantitative information
- c. Numeracy and calculation skills, including such aspects as error analysis, order-ofmagnitude estimations, and correct use of units
- d. Ability to use computers as information and research tools; Skills in informationretrieval and evaluation, in relation to primary and secondary information sources, including information retrieval through on-line computer and traditional library searches

- e. Interpersonal skills relating to the ability to interact with other people and to work in a team; ability to collaborate with other researchers
- f. Study and self-development skills needed for continuing professional development and life-long learning.
- g. Ability to exercise ethical principles and social responsibility in their professional and personal endeavors.

#### ARTICLE V CURRICULUM

#### Section 8 Curriculum Description

Chemistry is a central and essential science and is a fundamental part of many other disciplines. Therefore, the curriculum for B.S. Chemistry should be built around a well-defined core of subjects that covers the fundamental aspects in sufficient depth and at the same time allow for flexibility to cover areas and applications in the allied disciplines. The curriculum should also provide the necessary background in mathematics, physics, biology, information and computational sciences to prepare Chemistry graduates for higher levels of technical expertise.

The *Policies and Standards* makes the recommendations on about 80-85% of the Chemistry curriculum and the content of each course. The purpose of this is to ensure a common standard for the B.S. Chemistry degree. However, the individual Chemistry institutions are given the flexibility to offer courses and topics of their preference for the remainder of the curriculum and the course contents that are unspecified. It should be also emphasized that flexibility is allowed as long as the basic topics are covered.

All graduates from a BS Chemistry program should be competent in the following topics and skills:

- a. Major aspects of chemical terminology, nomenclature, conventions and units
- b. The structure and reactivity of the major classes of organic and inorganic compounds
- c. The major types of chemical reactions and the main characteristics associated with them
- d. The principles and procedures used in basic types of classical and instrumental chemical analysis
- e. Proper handling of numerical data, error, precision, estimation of error; principles of sampling
- f. The principal techniques of structural determination by spectroscopic techniques
- g. The characteristics of the different states of matter and the theories used to describe them
- h. The principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules
- i. The principles of thermodynamics and their applications to chemistry
- j. The kinetics of chemical change, including catalysis; the mechanistic interpretation of chemical reactions
- k. The characteristic properties of elements and their compounds, including group relationships and trends within the Periodic Table
- 1. The structural features of chemical elements and their compounds, including stereochemistry
- m. The properties and chemical reactivity of organic functional groups

- n. Basic synthetic strategies in organic chemistry, including catalysis
- o. The relation between bulk properties and the properties of individual atoms and molecules, including macromolecules (both natural and synthetic), polymers and other related materials
- p. Understand biological phenomena at the molecular level
- q. Awareness of current challenges and ethical issues in science, in general, and Chemistry, in particular
- r. Understand and practice Chemical safety and waste management
- s. Ability to think in an integrated manner and look at problems from different perspectives
- t. Ability to learn new chemistry and chemical techniques

As a minimum, the B.S. Chemistry degree should fulfill the requirements of the Chemistry Law (RA 754) of 60 units of chemistry and prepare the student to take the Chemistry Licensure Examinations.

## Section 9 Curriculum Components

The components of the BS Chemistry curriculum are listed in Table 1 below together with the minimum number of units in each component.

COMPONENTS		UNITS
General Education Curriculum		51
Core Courses		
Science and Math Component		13
Chemistry <sup>1</sup>		48
Electives <sup>1</sup>		6
Thesis/Professional Exposure <sup>1</sup>		6
	Total	124

Table1. Components of the BS Chemistry curriculum and their corresponding units.

<sup>1</sup>Credited towards the 60-unit board course requirement of the Chemistry Law.

## Section 10 General Education (GE) Courses (51 units)

The general education and legislated courses will follow the CHED Memorandum No. 04 series of 1997 (GEC-B; 51 units). The list of GE courses is in Table 2.

Table 2. GE courses and corresponding units	Table 2.	2. GE courses	and correst	ponding	units.
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FIELDS OF STUDY	SPECIFIC COURSES	Ul	NITS
1. Language and	English	6	21
Humanities	Filipino	6	
	Humanities Subjects (e.g. Literature, Art, Philosophy)	9	
2. Mathematics, Natural	Mathematics	6	15
Sciences and	Natural Science	6	
Information	Elective (e.g. Information Technology, STS)	3	
Technology			

Table 2 continued			
FIELDS OF STUDY	SPECIFIC COURSES	UN	NITS
3. Social Sciences	Consist of subjects such as Political Science, Psychology, Anthropology, Economics, History and the like, provided that the following topics are taken up in appropriate subjects: Taxation and Land Reform, Philippine Constitution, Family Planning and Population Education. Life and Works of Rizal <i>(Mandated Subject)</i>		15
		lotal	51

## Section 11 Core courses (73 units)

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## 11.1 Science and mathematics courses (25 Units)

The BS Chemistry program requires 25 units of non-chemistry core courses; 12 units of this requirement are fulfilled by the GE Natural Science and GE Mathematics courses. Table 3 lists the non-chemistry core courses that should be taken by students in the program. The minimum number of required units per area is also given in the table below.

Table 3. Non-chemistry core courses and corresponding units.

AREAS	COURSES	UNITS
Physics	Modern Physics (lec)	10
	Mechanics and Heat (lec/lab)	
	Electricity, Magnetism and Optics (lec/lab)	
Mathematics	Algebra	15
	Trigonometry	
	Analytic Geometry	
	Differential Calculus	
	Integral Calculus	

#### 11.2 Core Chemistry courses (48 Units)

The core chemistry courses are listed in Table 4 and their corresponding minimum number of units. An equivalent combination of lecture and laboratory courses may be offered provided the basic topics and skills in each core area are covered.

Table 4. List of chemistry core courses.

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COURSES		UNITS
General Chemistry 1 (lec/lab)		5
General Chemistry 2 (lec/lab)		5
Organic Chemistry 1 (lec/lab)		5
Organic Chemistry 2 (lec/lab)		5
Analytical Chemistry 1 (lec/lab)		5
Analytical Chemistry 2 (lec/lab)		5
Biochemistry (lec/lab)		4
Inorganic Chemistry (lec or lec/lab)		3
Physical Chemistry 1 (lec/lab)		4
Physical Chemistry 2 (lec/lab)		4
Physical Chemistry 3 (lec or lec/lab)		3
	Total	48

# Section 12 Chemistry Electives (6 Units)

The BS Chemistry curriculum includes Chemistry electives. The Chemistry department may wish to emphasize special areas of Chemistry through the electives.

In order to give maximum flexibility and to enable efficiency in the coverage of topics, the following measures are suggested:

- a. These electives should be taken towards the end of the student's course work. The treatment of these courses should include an in-depth discussion of all of the relevant principles in Organic, Inorganic, Physical Chemistry and Biochemistry rather than a superficial enumeration of their chemical aspects. In addition, these electives should integrate all of the necessary chemical principles so as to provide a coherent overview on the role of Chemistry in these important areas.
- b. These courses should cover on topics which are relevant to the Philippine situation when possible;
- c. These courses can be enriched by field visits and the participation of relevant experts in the course, such as a Chemical Engineer in the case of Industrial Chemistry, and an Agriculturist in the case of Agricultural Chemistry.
- d. The number of units assigned to the electives is left to the discretion of the institution.

ELECTIVE COURSE	PREREQUISITES
Advanced Organic Chemistry	Organic Chemistry 2
Advanced Biochemistry	Biochemistry
Advanced Inorganic Chemistry	Inorganic Chemistry
Advanced Analytical Chemistry	Analytical Chemistry 2
Materials Chemistry	Inorganic Chemistry and Organic Chemistry 2
Polymer Chemistry	Organic Chemistry 2; Physical Chemistry 2
Environmental Chemistry	Organic Chemistry 1; Analytical Chemistry 1
Natural Products Chemistry	Organic Chemistry 2; Biochemistry
Food Chemistry	Organic Chemistry 2; Biochemistry
Industrial Chemistry	Organic Chemistry 2; Inorganic Chemistry
Agricultural Chemistry	Organic Chemistry 2, Inorganic Chemistry
Computational Chemistry	Physical Chemistry 3
Advanced Physical Chemistry	Physical Chemistry 2 or 3

Table 5. List of suggested chemistry electives.

## Section 13 Thesis or Research and Professional Exposure (6 Units)

This component could be a thesis or a combination of thesis and on-the-job (OJT) training. HEIs shall have the prerogative to choose a mode of implementing this requirement based on the available resources within the institution and opportunities for collaboration with suitable outside organizations.

((Thesis = 6 units; (Thesis) + (OJT / practicum / professional exposure) = 6 units))

## Section 14 Sample Program of Study

The sample program of study and the recommended sequence of Chemistry, Physics and Mathematics courses is given in Table 6 below. Institutions may modify the curriculum

to suit their particular requirements and thrusts. Some courses, for example the mathematics courses, may be accelerated so that these are finished within the first 2 years. Institutions may choose to offer certain courses during the summer.

		τ	U <b>nit</b>	ts		τ	J <b>ni</b> t	s
Year	1st Semester Courses	Lec	Lab	Total	2nd Semester Courses	Lec	Lab	Total
Ι	General Chem 1	3	2	5	General Chem 2	3	2	5
	Algebra (GE Math 1)	3		3	Analytic Geometry	3		3
	Trigonometry (GE	3		3	GE course 3	3		3
	Math 2)	3		3	GE course 4	3		3
	GE course 1	3		3	GE course 5	3		3
	GE course 2		(2)	(2)	PE 2		(2)	(2)
	PE 1		(3)	(3)	NSTP 2		(3)	(3)
	NSTP 1							
		15	2	17		15	2	17
II	Analytical Chem 1	3	2	5	Organic Chem 1	3	2	5
	Differential Calculus	3		3	Integral Calculus	3		3
	Mechanics and Heat	3	1	4	Electricity, Magnetism &	3	1	4
	GE course 6	3		3	Optics			
	PE 3		(2)	(2)	GE course 7	3		3
	NSTP 3		(3)	(3)	PE 4		(2)	(2)
					NSTP 4		(3)	(3)
		12	3	15		12	3	15
III	Organic Chem 2	3	2	5	Biochem	3	1	4
	Analytical Chem 2	3	2	5	Physical Chem 2	3	1	4
	Physical Chem 1	3	1	4	Modern Physics	3		3
	GE course 8	3		3	GE course 9	3		3
					GE course 10	3		3
		12	5	17		15	2	17
IV	Physical Chem 3	3		3	Chem Elective 2	3		3
	Inorganic Chem	3		3	GE course 12	3		3
	Chem Elective 1	3		3	GE course 13	3		3
	GE course 11	3		3	Thesis 2	3		3
	Thesis 1	3		3				
		15		15		12		12

Table 6. Sample program of study and recommended sequence of chemistry, mathematics and physics courses.

## ARTICLE VI COURSE SPECIFICATIONS

#### Section 15 Core Chemistry Courses

The following course specifications apply only to the core courses and indicate the minimum topics to be covered in each area.

There are six core courses for the BS Chemistry Program: General Chemistry, Organic Chemistry, Analytical Chemistry, Inorganic Chemistry, Biochemistry, and Physical

Chemistry. In addition, the BS Chemistry program requires six (6) units of undergraduate thesis and professional exposure. There are six (6) units of elective courses.

It is suggested that the introductory and/or concluding part of each Chemistry course present an informative survey of advances and prospects in this area in order to elicit more interest from the student. While the course must continue to impart skills to the student, it should also try to sustain or increase the interest of the student in Chemistry.

# 15.1 GENERAL CHEMISTRY

## INTRODUCTION TO SUBJECT AREA

General Chemistry is the first required course for the BS Chemistry major. It is a twosemester introductory course on the fundamental concepts and principles of chemistry. The topics covered are the structure and properties of matter, the energetics of chemical reactions, and the equilibrium and kinetic aspects of chemical reactions.

This course should develop a deeper appreciation for Chemistry, a greater sense of excitement in discovery, and a stronger commitment to master the fundamental skills.

## **OBJECTIVES OF SUBJECT AREA**

- a. To provide an introduction to the basic concepts and principles that will be needed in the higher chemistry courses.
- b. To demonstrate how essential chemical principles are applied to rationalize experimental observations and to predict and control the behavior of matter.
- c. To present the macroscopic-microscopic paradigm of chemistry, wherein macroscopic properties are understood through microscopic, molecular and atomic structures.
- d. To introduce the methods and techniques of scientific investigation, leading to the development of research skills that will be needed in the higher chemistry courses.
- e. To link chemical concepts and principles with practical application and the life experiences of the student.
- f. To train the student to work independently and as an active member of a group. This can be implemented by requiring individual work, and where appropriate, group work, both in the lecture and laboratory courses.
- g. To provide the student with an environmental perspective on the role of chemistry in meeting the needs of society.

## 15.1.1 GENERAL CHEMISTRY 1

#### **COURSE DESCRIPTION**

This is the first part of a two-semester course on the fundamental chemical concepts and principles that covers the structure of matter; atomic structure and chemical bonding; and chemical reactions: classification, stoichiometry and energetics.

NUMBER OF UNITS: 3 units

**PREREQUISITE:** None

# **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Describe matter and its structure, in terms of atoms, ions and molecules
- b. Explain and predict the behavior of simple atoms and molecules in terms of their electronic structure and interactions
- c. Describe quantitatively chemical reactions and perform calculations involving the application of chemical principles
- d. Discuss how energy is involved in physical and chemical changes

# **COURSE OUTLINE**

# a. Introduction (2 hours)

Chemistry: definition and scope. The scientific method: laws and theories. Matter: classification and physical states; physical and chemical properties. Measurement: units and handling numbers. Problem solving; dimensional analysis / factor-label method.

# b. Atoms, Ions and Molecules (2 hours)

Atomic theory. Structure of the atom: nucleus and electrons; atomic number and mass number; isotopes. Ions: cations and anions. Molecules. Chemical formulas. Naming compounds.

# c. Mass Relationships in Chemical Reactions (6 hours)

Atomic mass. Molar mass. Avogadro's number. Percent composition of compounds. Calculation of empirical formulas. Chemical reactions and chemical equations. Amounts of reactants and products. Limiting reagents. Percent yield of reactions.

# d. <u>Electronic Structure of Atoms (6 hours)</u>

Development of the quantum theory: Planck theory; photoelectric effect; Bohr theory; dualism principle. Quantum mechanics: Schrödinger equation. Quantum numbers. Atomic orbitals. Electronic configuration. Aufbau principle. Pauli exclusion principle. Hund's rule.

## e. Periodic Relationships among Elements (3 hours)

Development of the periodic table. Periodic classification of elements. Periodic variation of properties: nuclear charge; atomic size; ionization energy; electronic affinity; chemical properties.

# f. <u>Chemical Bonds – Basic Concepts (3 hours)</u>

Lewis dot symbols. Ionic bonds. Lattice energy. Covalent bonds. Electronegativity. Lewis structures: octet rule. Bond strength.

## g. Chemical Bonding: Molecular Geometry and Molecular Orbitals (6 hours)

Molecular geometry. VSEPR model. Valence Bond Theory. Hybrid orbitals, multiple bonds. Basic Molecular Orbital Theory. Bonding and anti-bonding orbitals. Electronic configuration.

## h. <u>Reactions in Aqueous Solutions (3 hours)</u>

Solutions and solubility. General properties of aqueous solutions. Electrolytes and nonelectrolytes. Precipitation reactions. Acid-base reactions. Oxidation-reduction reactions. Chemical analysis: gravimetric methods; titration and volumetric methods.

# i. <u>Chemical Thermodynamics (4 hours)</u>

Energy.Energy changes in chemical reactions: enthalpy. Calorimetry. Thermochemistry: standard enthalpy; heat of fusion, heat of vaporization, heat of solution, heat of reaction. First law of thermodynamics. Spontaneity of processes.

# j. Gases (4 hours)

Nature of gases. Gas laws: Boyle's law; Charles law; Avogadro's law; Ideal gas law. Gas mixtures.: Dalton's law of partial pressure. Stoichiometry involving gases. Kinetic molecular theory of gases. Deviation from ideal behavior. Real gases.

# k. Intermolecular Forces: Liquids and Solids (4 hours)

Kinetic molecular theory of liquids and solids. Intermolecular forces. Properties of the liquid state: surface tension, viscosity. Crystal structure. Boiling points. Melting points. Phase changes. Phase diagrams. Colloids.

## **COURSE DELIVERY**

A combination of the traditional lecture approach, use of models and demonstrations, web-enhanced learning, computer-aided learning and learner-centered activities, such as structured exercises, team projects and group discussions.

## SUGGESTED TEXTBOOKS

Whitten, K.W., Davis, R.E., Peck, M.L. and Stanley, G. G. (2004) *General Chemistry*, 8<sup>th</sup> ed., Thomson Brooks/Cole (or latest edition).

Silberberg, M.S. (2003) Chemistry – The Molecular Nature of Matter and Change,  $3^{nd}$  ed., McGraw-Hill (or latest edition).

Brown, T.L., LeMay Jr., H.E. and Bursten, B.E. (2005) *Chemistry – The Central Science*,  $10^{th}$  ed., Prentice-Hall International, Inc (or latest edition).

Chang, R. (2005) Chemistry, 8th ed., McGraw-Hill (or latest edition).

Masterton, W.L. and Hurley, C.N. (2004) Chemistry – Principles and Reactions,  $5^{tb}$  ed., Thomson Brooks/Cole (or latest edition).

# 15.1.2 GENERAL CHEMISTRY 2

## **COURSE DESCRIPTION**

General Chemistry 2 is the second part of a two-semester course on the fundamental chemical concepts and principles, including solutions, chemical kinetics, chemical equilibria, electrochemistry, nuclear chemistry and descriptive chemistry of metals, nonmetals and the transition elements.

NUMBER OF UNITS: 3 units

**PREREQUISITE:** General Chemistry 1

## **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Discuss the principles involved in the formation of solutions and describe the properties of solutions;
- b. Explain the kinetics and equilibrium aspects of chemical reactions;
- c. Understand the principles of an electrochemical cell and describe its properties;
- d. Discuss the properties and behavior of metals, nonmetals and transition elements;

- e. Apply chemical principles to explain various chemical phenomena;
- f. Perform calculations involving the application of chemical principles;
- g. The student should be able to relate all of these principles to everyday phenomena and to practical applications.

## **COURSE OUTLINE**

## a. Physical Properties of Solutions (5 hours)

Definition and properties of solutions. Types of solutions. The solution process. Concentration units. Factors affecting solubility: structure, temperature, pressure. Colligative properties. Nonelectrolytes. Electrolytes. Colloids.

## b. Chemical Kinetics (5 hours)

The rate of a reaction. Rate laws. Order of reaction. Temperature dependence of reaction rates. Collision theory. Activation energy. Catalysis.

## c. <u>Chemical Equilibrium (5 hours)</u>

The concept of equilibrium. Equilibrium constant. Calculation. Significance. Factors affecting equilibrium: Concentration changes. Pressure changes. Temperature changes. Catalysts.

## d. Acids and Bases (5 hours)

Concepts of acids and bases. Arrhenius concept. Bronsted concept. Lewis concept. Acid-base properties of water. pH. Weak acids and bases. Ionization constants. Strength of acids and bases. Diprotic and polyprotic acids. Typical acid-base reactions. Acid-base properties of salts. Hydrolysis. Introduction to non-aqueous acid and base systems.

## e. Acid-Base and Solubility Equilibria (5 hours)

Homogeneous and heterogeneous equilibria. Common-ion effect. Buffer solutions. Solubility and solubility product. Fractional precipitation. Factors affecting solubility. Common ion effect. pH.

#### f. Electrochemistry (5 hours)

Redox reactions. Galvanic cells. Electrode reactions. Cell emf. Standard electrode potentials. Effect of concentration. Nernst equation. Practical electrochemistry. Batteries. Corrosion. Electrolysis.

#### **OPTIONAL TOPICS:**

## g. Metallurgy and the Chemistry of Metals (3 hours)

Occurrence of metals. Metallurgical processes. Band theory of conductivity. Semiconductors. Properties of metals. Alkali metals. Alkaline earth metals.

#### h. Nonmetallic Elements and Their Compounds (3 hours)

General properties of nonmetallic elements. Properties of nonmetals. Hydrogen. Carbon. Nitrogen and phosphorus. Oxygen and sulfur. Halogens.

#### i. <u>Transition elements (4 hours)</u>

General properties of the transition elements. Coordination compounds: structure and reactions.

# j. Nuclear Chemistry (4 hours)

Nuclear reactions. Nuclear stability. Natural radioactivity. Kinetics of nuclear decay. Nuclear transmutation. Nuclear fission. Nuclear fusion. Uses of isotopes. Biological effects of radioactivity.

## SUGGESTED TEXTBOOKS

Whitten, K.W., Davis, R.E., Peck, M.L. and Stanley, G.G. (2004) *General Chemistry*, 8<sup>th</sup> ed., Thomson Brooks/Cole (or latest edition).

Silberberg, M.S. (2003) *Chemistry.* The Molecular Nature of Matter and Change, 3<sup>rd</sup> ed., McGraw-Hill (or latest edition).

Brown, T.L., LeMay Jr., H.E. and Bursten, B.E. (2005) *Chemistry – The Central Science, 10<sup>th</sup> ed.*, Prentice-Hall International, Inc (or latest edition).

Chang, R. (2005) Chemistry, 8th ed., McGraw-Hill (or latest edition).

Masterton, W.L. and Hurley, C.N. (2004) *Chemistry – Principles and Reactions*,  $5^{tb}$  ed., Thomson Brooks/Cole (or latest edition).

## 15.1.3 GENERAL CHEMISTRY LABORATORY

## **COURSE DESCRIPTION**

The General Chemistry Laboratory 1 & 2 courses introduce the student to the fundamental techniques and skills needed in the Chemistry laboratory. It emphasizes the formation of proper practices and habits, including laboratory and chemical safety, waste minimization and proper and efficient use of resources, and the preparation of proper laboratory reports.

## NUMBER OF UNITS

General Chemistry 1 Laboratory: 2 units General Chemistry 2 Laboratory: 2 units

#### REQUISITES

<u>General Chemistry 1 Laboratory</u> Co-requisite: General Chemistry 1 Lecture

<u>General Chemistry 2 Laboratory</u> Co-requisite: General Chemistry 2 Lecture Prerequisite: General Chemistry 1 Laboratory

## **COURSE COMPETENCIES:**

At the end of the General Chemistry laboratory course series, the student should be able to:

- a. Exhibit mastery of basic laboratory techniques;
- b. Make valid observations and perform reliable and reproducible measurements;
- c. Analyze experimental data and interpret them correctly applying appropriate chemical principles and mathematical techniques;
- d. Develop the techniques necessary to attain accuracy and precision;
- e. Apply basic statistical methods of analysis in the evaluation of experimental data;
- f. Prepare an accurate record and a proper scientific report of the results of an experiment;
- g. Identify safety requirements and perform laboratory exercises safely;

- h. Make efficient use of the laboratory materials, minimize waste and store and dispose of chemicals properly;
- i. Demonstrate systematic and logical approaches in solving practical problems in chemistry using the principles of qualitative and quantitative analysis; and
- j. Apply the principles of ethics and truth in science.

## **RECOMMENDED TOPICS FOR LABORATORY ACTIVITIES**

- a. Scientific method: observing and data gathering, data analysis and interpretation, making conclusions.
- b. Classification of matter
- c. Composition of compounds
- d. Mole concept
- e. Stoichiometry
- f. Thermochemistry
- g. Rates of reactions
- h. Oxidation-reduction reactions
- i. Periodicity of properties
- j. Geometry of molecules
- k. Intermolecular forces of attraction
- 1. Changes of state: Cooling and heating curves
- m. Chemical equilibrium and Le Chatelier's Principle
- n. Properties of solutions; colligative properties
- o. Determination of solubility product constant
- p. Acid-base equilibrium, buffers
- q. Exercises on qualitative analysis

#### SAMPLE EXPERIMENTS AND TECHNIQUES

Table 7 lists the recommended minimum topics for the course and the techniques to be learned. Various topics can be covered by more than one experiment. The experiments may be timed to match the topics covered in the lecture classes. The first two exercises must be done before the other experiments. The other experiments may be done in any sequence.

Institutions are encouraged to use microscale experiments and low cost/fabricated equipment.

	Topics	Sample Experiments	Lab Techniques Involved
1	Introduction / Lab safety and Waste Management	Demonstrations Film showing Exercises Use of MSDS Proper laboratory attire Proper use of laboratory notebook	<ul> <li>Handling of hazardous chemical reagents and wastes</li> <li>First aid procedures</li> <li>Fire and earthquake drills</li> </ul>
2	Measurement	Density of liquids and solids	<ul> <li>Cleaning glasswares</li> <li>Handling solid and liquid reagents</li> <li>Weighing / volume</li> </ul>

Table 7. Sample experiments and techniques to be learned for General Chemistry 1 & 2 Laboratory.

	Topics	Sample Experiments	Lab Techniques Involved
3	Stoichiometry	<ul><li>a) Determination of molecular formula</li><li>b) Volumetric analysis</li></ul>	<ul> <li>Care and manipulation of the balance Significant figures from measurements and calculations</li> <li>Reading and recording meniscus</li> <li>a) Weighing</li> <li>b) Titration</li> <li>Using a crucible</li> <li>Using a Bunsen burner</li> <li>Vacuum filtration (Buchner)</li> <li>Preparing solutions</li> <li>Handling of burets and</li> </ul>
4	Electronic	Atomic spectra	other volumetric glassware Flame test or Emission
5	structure Periodic Table	Periodicity of properties of elements	<ul> <li>spectroscopy</li> <li>Microscale techniques / chemical handling</li> <li>Measurement of acidity</li> </ul>
6	Chemical reactions	a) Reactions between ions b) Redox reactions	<ul> <li>and basicity</li> <li>Conductivity measurement</li> <li>Microscale techniques of preparing electrochemical cells / Chemical handling</li> </ul>
7	Thermochemistry	Heat of reaction	<ul> <li>Calorimetry / Microscale Techniques</li> </ul>
8	Gases	Molar mass of a volatile liquid	<ul> <li>Weighing</li> <li>Handling glassware</li> <li>Water displacement</li> <li>Venting gases</li> </ul>
9	Phase changes	Temperature behavior during solid-liquid transition	• Temperature reading / Graphical analysis
10	Solutions	a) Conductance of solutions	a) Conductimetry b) Weighing c) Temperature reading
11	Intermolecular forces	<ul> <li>b) Temperature effects on solubility / crystallization</li> <li>c) Cryoscopic method for the determination of molar mass</li> <li>Solubility classification</li> <li>TLC, paper chromatography</li> </ul>	<ul><li>Preparing solutions</li><li>Use of water bath</li><li>Crystallization</li></ul>

	Topics	Sample Experiments	Lab Techniques Involved
12	Chemical Kinetics	Rate measurements a) Iodine clock reaction b) Iodide-iodate reaction c) Crystal violet oxidation	a) Dilution / graphical analysis b) Colorimetry
13	Chemical Equilibrium	<ul><li>a) Determination of K</li><li>b) Le Chatelier principle</li></ul>	Colorimetry
14	Acids and Bases	<ul><li>a) Volumetric analysis</li><li>b) pH measurement</li><li>c) Standardization using primary standards</li></ul>	<ul><li>a) Titration</li><li>b) Use of pH meter</li><li>Drying using an oven or a desiccator</li></ul>
15	Ionic Equilibrium (Acid-Base / Solubility)	a) Determination of pK b) Buffers	<ul> <li>a) Colorimetry / potentiometry</li> <li>b) Potentiometry</li> <li>Preparation of a buffer solution</li> </ul>
16	Electrochemistry	Electrochemical cells / Nernst equation	• Potentiometry (low-cost) / electronics
17	Metals	<ul><li>a) Reactions of cations</li><li>b) Qualitative analysis of cations</li></ul>	<ul> <li>Handling of chemicals / centrifugation</li> <li>Filtration</li> <li>Decantation</li> </ul>
18	Nonmetals	<ul><li>a) Reactions of anions</li><li>b) Qualitative analysis of anions</li></ul>	<ul> <li>Handling of chemicals / centrifugation</li> <li>Filtration</li> <li>Decantation</li> </ul>
19	Transition elements	a) Determination of formula of coordination compounds b) Volumetric analysis	a) Colorimetry b) Titration

#### SUGGESTED TEXTBOOKS

Table 7. continued

Slowinski, E.J., Wosley, W.C. and Masterton, W.L. (2005) Chemical Principles in the Laboratory, 8th ed., Brookes/Cole, USA (or latest edition).

Beran, J.A. (2004) Laboratory Manual for Principles of General Chemistry, 7th ed., John-Wiley & Sons, USA (or latest edition).

## 15.2 ORGANIC CHEMISTRY

#### INTRODUCTION

The scope of topics proposed here is considered as the minimum requirement for chemistry students to prepare them for a career in chemistry.

## **OBJECTIVES OF SUBJECT AREA**

The core courses in organic chemistry subject area provide the basic knowledge needed for a wide range of topics. The overall objectives of the subject area include the following:

- a. To understand organic structure and its relationship to chemical properties and reactivity;
- b. To gain an in-depth understanding of importance and impact of organic chemistry in industry, the environment, agriculture, medical and pharmaceutical sciences, and others;
- c. To demonstrate and apply modern theories in the organic chemistry laboratory;
- d. To introduce the principles of chemical waste minimization and management as a general principle in the manufacture, use and disposal of organic compounds; to apply the principles of environmental responsibility in particular with respect to organic chemistry.

## ORGANIC CHEMISTRY 1 AND 2: FUNDAMENTALS OF ORGANIC CHEMISTRY

## **COURSE DESCRIPTION**

Basic Organic Chemistry is made up of two semesters of lectures. There are two approaches that may be used:

- a. By functional groups: The two courses cover the functional groups sequentially in order of increasing complexity. The structure, stereochemistry, nomenclature, chemical properties, reactivity, basic synthesis and spectroscopic analysis of each functional group are covered together.
- b. Structure and reactivity: The first semester covers organic structure, stereochemistry, nomenclature and spectroscopic analysis, while the second semester shall focus on chemical properties, reactivity and basic synthesis.

Regardless of the approach, all of the topics should have been covered at the end of two courses.

#### NUMBER OF UNITS

Organic Chemistry 1: 3 units Organic Chemistry 2: 3 units

#### REQUISITES

Organic Chemistry 1 Prerequisite: General Chemistry 2 Lecture and Laboratory

Organic Chemistry 2 Prerequisite: Organic Chemistry 1 Lecture and Laboratory

#### **COURSE COMPETENCIES**

At the end of the course, the students should be able to:

- a. Apply the concepts of organic structural theory to explain and predict the physical properties and chemical reactivity of organic molecules ranging from simple organic compounds to macromolecules and biomolecules;
- b. Recognize stereochemical differences, i.e. subtle differences in the three-dimensional structure of organic molecules which affect optical, physical and chemical properties; assign the configuration at each chiral center in an asymmetric molecule;
- c. Use molecular modeling software for conformational analysis and stereochemical analysis of chiral compounds;

- d. Identify organic compounds, give their IUPAC names, and draw the molecular structures of these compounds;
- e. Identify the organic starting material, organic product and/or necessary reagents for chemical reactions that are characteristic of the different functional classes of organic compounds;
- f. Write out the detailed reaction mechanisms of common organic reactions;
- g. Analyze organic reactions using structural, mechanistic, thermodynamic and kinetic considerations;
- h. Map out strategies for the synthesis of organic compounds from simpler starting materials;
- i. Apply chemical methods and spectroscopic techniques such as UV-visible, IR, NMR and MS for the analysis of simple organic compounds; and
- j. Understand and practice chemical safety and waste minimization.

## COURSE OUTLINE

The topics enumerated below are expected to be taken up within two semesters. The following recommended list of topics indicates the number of hours that might be spent on the various topics. Inclusion of additional topics is left to the discretion of the lecturer.

The lecturer is given the option to arrange the sequence of topics to be discussed. Lecturers should use teaching aids such as molecular models and molecular modeling software in order to stimulate the interest of the students and facilitate learning especially abstract concepts. If possible, film features illustrating the relevance of organic chemistry to everyday life in modern society should also be shown as part of the lecture. Internet access is strongly recommended.

## a. Introduction (12 hours)

This includes a review of topics in general chemistry that are necessary for the understanding of organic chemistry: atomic structure, ionic vs. covalent bonds, electron accounting and Lewis structures of organic molecules (including isomeric and resonance structures), basic M.O. and valence bond theory, types of covalent bonds, properties of covalent bonds, hybridization and the geometry and shape of simple organic molecules, intermolecular and intramolecular attractive forces, Lewis and Brönsted-Lowry acids and bases.

Additional topics may include functional groups and the classification scheme for organic compounds; types of reactions based on net transformation (substitution, addition, elimination, oxidation and reduction, rearrangement); types of reaction mechanisms, bond cleavage and reactive intermediates; reaction energetics.

## b. <u>Stereochemistry (9 hours)</u>

Topics include optical activity and chirality; types of configurational isomers (enantiomers, diastereomers, and *meso* compounds), racemic mixtures; use of stereochemical drawings (flying wedge, Fischer, Newman and sawhorse projections); molecular configuration (R and S designations); conformations and conformational analysis. Relevance to biological activity (e.g. drugs, flavor compounds and agrochemicals) and polymer properties (tacticity) should be emphasized. A programmed learning module using SPARTAN/SPARTANVIEW, CHEM3D, or PCMODEL may be included to introduce the students to molecular modeling as a tool for the study of stereochemistry.

# c. Chemistry of the Different Classes of Organic Compounds (42 hours)

The different classes of organic compounds based on their functionality are enumerated below. Their discussions should include its nomenclature, physical properties, sources, uses, preparation, analysis, reactions and mechanisms.

- Alkanes, alkenes, alkynes and polyenes
- Alicyclic and cyclic hydrocarbons
- Alkyl halides
- Alcohols, ethers and epoxides
- Carboxylic acids and derivatives
- Aldehydes and ketones
- Benzene and aromatic derivatives
- Phenols
- Amines
- Polyfunctional compounds
- Introduction to Biomolecules: fats, carbohydrates, amino acids and proteins

## d. Spectroscopy (9 hours)

Lecture topics include basic theory of UV-visible, nuclear magnetic resonance, infrared, and mass spectroscopy and its applications to simple organic molecules.

## e. Synthesis (9 hours)

Previously discussed organic chemical reactions are applied to simple multi-step synthesis problems.

# f. Introduction to Waste Minimization and Management of Organic Chemicals (2 hours)

## SUGGESTED Textbooks.

McMurry, J. (2003) Organic Chemistry, 6th ed., Thomson Learning.

Brown, W. and Foote, C. (2002) Organic Chemistry, 3rd ed., Thomson Learning.

Wade Jr, L.G. (2005) Organic Chemistry, 6th ed., Prentice Hall.

Solomons, G. and Fryhle, C. (1999) Organic Chemistry, 7<sup>th</sup> ed., John Wiley & Sons (or latest edition).

Carey, F. (2003) Organic Chemistry, 5th ed., McGraw Hill.

Vollhardt, P., Shore, N., Freeman, W. (1998) Organic Chemistry, 3<sup>rd</sup> ed., W.H.Freeman & Co Ltd.

Morrison, R. T. and Boyd, R. N. (1999) Organic Chemistry, 6<sup>th</sup> Package ed., Prentice Hall College Division.

Brown, W. H. (2004) Organic Chemistry

Loudon, G. M. (2001) Organic Chemistry,4<sup>th</sup> ed., Oxford University Press, USA.

Streitwieser, A. and Heathcock, C. H. (1994) Introduction to Organic Chemistry, 4<sup>th</sup> ed., Prentice Hall (or latest edition).

## 15.2.1 ORGANIC CHEMISTRY 1 AND 2 LABORATORY

## **COURSE DESCRIPTION**

The Organic Chemistry 1 & 2 Laboratory courses equip the student with the basic laboratory procedures and skills of Organic Chemistry. It is concerned with the formation of proper practices and habits, including laboratory and chemical safety, waste minimization and proper and efficient use of resources, and the preparation of proper laboratory reports.

# NUMBER OF UNITS

Organic Chemistry 1 Laboratory: 2 units Organic Chemistry 2 Laboratory: 2 units

# REQUISITES

Organic Chemistry 1 Laboratory

Prerequisite:General Chemistry 2 Lecture and LaboratoryCorequisite:Organic Chemistry 1 Lecture

Organic Chemistry 2 Laboratory

Prerequisite:Organic Chemistry 1 Lecture and LaboratoryCorequisite:Organic Chemistry 2 Lecture

# **COURSE COMPETENCIES**

At the end of the laboratory course, the students should be able to:

- a. Isolate and purify organic compounds;
- b. Synthesize simple organic compounds through the application of organic reactions;
- c. Analyze and identify the structure of simple organic compounds; and
- d. Practice safety precautions in the laboratory.

# **Recommended Topics for Laboratory Activities**

The recommended topics are listed below. Table 8 shows the sample laboratory experiments and mode of delivery.

- a. Extraction
- b. Melting Point and Boiling Point Determination
- c. Distillation (at least 2 types of set-up)
- d. Crystallization
- e. Sublimation
- f. Chromatography (TLC and Gravity (open) column)
- g. Elemental Analysis of Organic Compounds
- h. Functional Group Analysis of Organic Compounds
- i. Systematic Identification of Organic Compounds
- j. Acid Catalyzed Dehydration of Alcohols
  - Cyclohexene from Cyclohexanol
  - Pentenes from 2-Pentanol
- k. Nucleophilic Substitution Reaction, Second Order
  - Conversion of 1-Butanol to 1-Bromobutane
  - 1 -Iodohexane from 1-bromohexane
- 1. Nucleophilic Substitution Reaction, First Order
  - Conversion of t-Amyl Alcohol to t-Amyl Chloride Using HCI
  - Kinetic Study of the Hydrolysis of t-Butyl Chloride
- m. Stereochemistry
  - Bromination of *cis* and *trans* stilbene
  - Diels-Alder Reaction of Conjugated Diene of Eucalyptus Oil
- n. Oxidation Reaction
  - Oxidation of Heptanal to Heptanoic Acid
  - o-Chlorotoluene to o-Chlorobenzoic Acid
- o. Electrophilic Aromatic Substitution Reaction

- Nitration of Methyl Benzoate
- Friedel-Crafts Alkylation of p-Dimethoxybenzene
- p. Ester Formation
  - Synthesis of Aspirin
  - Preparation of Isoamyl Acetate
- q. Condensation Reaction
  - Aldol Condensation of Acetone and Bensaldehyde
  - Claisen Condensation of Ethyl Acetate and Benzaldehyde
- r. Multiple Synthesis
  - Synthesis of Triphenylmethanol by Reaction of Methyl Benzoate and Phenylmagnesium Bromide

Table 8. Sample laboratory experiments and mode of delivery for organic chemistry 1 and 2 laboratory.

Experiment*	Mode of Deliverv**		
Experiment	Activities	Techniques	
<ol> <li>Orientation, Lab Safety Overview and Waste Treatment Management in the Laboratory</li> <li>Transfer and Extraction Technique</li> </ol>	- demonstration by video and laboratory orientation by instructor	- as shown in video	
(Hands on)	- manipulation and purification of known amount of contaminated material	<ul> <li>extraction and washing</li> <li>transfer without loss of material</li> <li>solvent drying and concentration</li> <li>mp determination</li> <li>interpretation of NMR spectra</li> </ul>	
Additional knowledge (e.g., Video only)	- manipulation of air sensitive sample w/o allowing sample to decompose	<ul> <li>cannula transfer</li> <li>vacuum manifold use</li> <li>manipulations under inert atmosphere</li> <li>solvent degassing</li> <li>air sensitive techniques</li> </ul>	
3. Purification of Solids by		1	
Recrystallization (Hands On)	- purification of a compound by recrystallization	<ul> <li>solubility test</li> <li>choosing a good solvent</li> <li>system</li> <li>inducing crystallization</li> <li>filtration</li> </ul>	
Additional knowledge (Video only)	- Separation of S from R enantiomer of a racemic material by use of two solvent system recrystallization	<ul> <li>two solvent system</li> <li>recrystallization</li> <li>HPLC using chiral column</li> </ul>	

Table 8 continued

Experiment*	Mode of Delivery**	
1	Activities	Techniques
4. Purification of Liquids by Distillation		
(Hands On)	- purification of a mixture of two liquids using distillation	- distillation set-up - atmospheric pressure and fractional distillation
Additional knowledge (Video only)	- purification of a mixture of two known liquids by reduced pressure distillation	<ul> <li>use of GC to analyze samples</li> <li>glassware set-up for reduced pressure distillation</li> <li>running reduced pressure distillation</li> </ul>
5. Purification by Flash		
Column Chromatography (Hands On)	- purification of a contaminated compound using silica gel flash chromatography	<ul> <li>TLC analysis</li> <li>silica gel column assembly</li> <li>sample application on silic gel column</li> <li>separating simple mixtures</li> </ul>
Additional knowledge (Video only)	- separation of a complex mixture of three compounds using gradient elution flash	<ul> <li>scparating simple initiales</li> <li>with silica gel column</li> <li>chromatography</li> <li>choosing the correct eluen</li> <li>adsorption of a crude</li> <li>mixture on silica gel</li> <li>use of gradient elution</li> </ul>
	column chromatography	- use of gradient elution
6. Free Radical Substitution		
Ex. Halogenation of 1- chlorobutane	- halogenation of alkane	<ul> <li>use of gas traps (SO<sub>2</sub>, HCl</li> <li>detn. of product ratio by</li> <li>GC</li> <li>liquid-liquid extraction</li> </ul>
7. Electrophilic Addition on		1 1
Alkene Ex. Bromination of <i>cis</i> - and <i>trans</i> -stilbene 8. Diels-Alder Reaction	- bromination of an alkene	- vacuum filtration - mp determination
Ex. Diels-Alder Reaction of Conjugated Diene of Eucalyptus Oil	- Diels-Alder reaction	<ul> <li>identification of functional groups by IR</li> <li>GC technique for separation of isomer</li> <li>mp determination</li> <li>molecular modeling</li> </ul>
9. Elimination Reaction Ex. Dehydration of Cyclohexanols (2- and 4- methylcyclohexa -nol)	- acid catalyzed dehydration of alcohols to cyclohexene	<ul><li>simple distillation</li><li>determination of product</li><li>ratio by GC</li></ul>

Table 8 continued

Experiment*	Mode of Delivery**			
1	Activities	Techniques		
10. Nucleophilic Substitution Reaction				
Ex.1 Synthesis of propyl p- tolylether (2 <sup>nd</sup> order)	- Williamson ether synthesis (S <sub>N</sub> 2)	<ul> <li>liquid-liquid separation</li> <li>HNMR technique</li> <li>drying of solution</li> </ul>		
Ex. 2 Synthesis of t-Butyl chloride (1 <sup>st</sup> order)	- reaction of a $3^{\circ}$ alcohol with HCl ( $S_{N}1$ )	- liquid-liquid separation - simple distillation - IR technique		
11. Nucleophilic Addition on Carbonyl Group				
Ex. Grignard Synthesis of Triphenylmethanol from Methylbenzoate 12. Oxidation-Reduction Reaction	- Grignard synthesis	<ul><li>no air and moisture</li><li>technique</li><li>mp determination</li></ul>		
Ex. Borohydride Reduction of a Benzil to hydroxy benzoin	- reduction of aldehydes and ketones	- mp determination		
Ex. Oxidation of Isoborneol to Camphor with Household Bleach	- oxidation of alcohol to aldehyde or ketone	- sublimation - IR technique -use of green reagent		
13. Electrophilic Substitution Reaction				
Ex. Friedel-Crafts Acylation of Ferrocene	- acetylation of an aromatic compound	<ul> <li>TLC technique (for monitoring reaction)</li> <li>recrystallization</li> <li>mp determination</li> </ul>		
Ex. Synthesis of Azo Dyes	-diazotization/coupling	<ul> <li>vacuum filtration</li> <li>dying of cloth</li> <li>possible combinatorial synthesis</li> </ul>		
14. Ester Formation		1,		
Ex. Synthesis of Cholesteryl Benzoate	- synthesis of a liquid crystal	-mp determination -recrystallization - liquid crystal property observation		
Ex. Synthesis of Aspirin	- synthesis of a pain reliever	- mp determination - recrystallization		
15. Condensation Reaction				
Ex. Aldol Condensation of a)Benzaldehyde with Acetone b)Acetaldehyde with acetone	- aldol condensation followed by dehydration of product	-recrystallization - mp determination		
16. Multiple Synthesis	- any three or more step synthesis, e.g., peptide synthesis	- techniques on separation, purification, spectroscopic identification, mp/bp etc., learned in preceding experiments		

Exposition on t*	Mode of Delivery**			
Experiment*	Activities	Techniques		
17. Elemental Analysis of	- use of sodium fusion	- elemental analyzer		
Organic Compounds	or elemental analyzer	techniques		
	methods	- elemental analysis by mass spectrometry		
18. Functional Group	- solubility classification,	- mp determination		
Analysis of Organic	functional group tests	- bp determination		
Compounds	and ignition test			
Ex. Two Unknowns (one	- observation of physical	- IR spectroscopy		
liquid, one solid or one acid,	properties, elemental	- NMR spectroscopy		
one neutral, etc.)	analysis, solubility test,	- optional UV spectroscopy		
	functional group	- optional GC-MS		
	classification	- mp determination		
	test,spectral analysis and			
	derivative synthesis			

#### Table 8 continued

# 15.3 ANALYTICAL CHEMISTRY

## INTRODUCTION

Analytical Chemistry 1 and 2 are designed to be problem-driven and emphasize critical thinking. It should be supplemented with topics that are relevant to the practice of chemistry, as well as those that students confront in their lives.

## **OBJECTIVES OF SUBJECT AREA**

The courses covered by the Analytical Chemistry subject area provide the basic methods and skills needed in the more advanced courses, as well as in industry. The overall objectives of the subject area include the following:

- a. To acquire mastery of the principles and practice of quantitative chemical analysis;
- b. To obtain a working knowledge of the applications of statistics in Analytical Chemistry; and
- c. To gain an in-depth understanding of the applications of Analytical Chemistry in industry, agriculture, molecular biology, medical sciences, and others.

## COMMENTS

The undergraduate Analytical Chemistry curriculum has undergone a number of developments during the past decades. The international trend in the teaching of analytical chemistry involves a shift from a superficial and comprehensive coverage of methods to the utilization of selected methods in the context of problem solving and quality assurance.

The course outlines for Analytical Chemistry 1 and 2 were based on the recommended content of the compulsory basic parts of Eurocurriculum II for Analytical Chemistry. The Eurocurriculum II for Analytical Chemistry emphasized that a sustainable curriculum in analytical chemistry requires orientation towards analytical fundamentals which are based on real-life applications.

# 15.3.1 ANALYTICAL CHEMISTRY 1: FUNDAMENTALS OF ANALYTICAL CHEMISTRY

#### **COURSE DESCRIPTION**

This course is designed to give students an understanding of the principles and practice of gravimetric and volumetric methods, potentiometry and spectrophotometry, analytical measurements and data analysis.

#### NUMBER OF UNITS: 3 units

**PREREQUISITE:** General Chemistry 2 Lecture and Laboratory

## **COURSE OBJECTIVES**

- a. To provide a strong foundation of chemical principles which are essential to the understanding of analytical chemistry;
- b. To introduce the fundamental concepts of sampling in chemical analysis;
- c. To present various classical and instrumental methods of chemical analysis;
- d. To apply statistics in evaluating the quality of analytical data;
- e. To develop critical thinking needed to solve analytical problems.
- f. To develop an appreciation for the role of analytical chemistry in various aspects of human life.

## **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Apply chemical principles in solving problems in quantitative chemical analysis.
- b. Integrate the use of classical chemical analysis in real-world problems.
- c. Apply statistics in evaluating quality of analytical data.

## **COURSE TOPICS**

The following topics should be discussed using a combination of traditional lecture and problem-based learning approach as teaching method. Real-life situations and contextual examples should be incorporated in the discussion of topics. Supplementary reading materials on emerging technologies related to the topics should be assigned.

## a. Introduction (1.5 hours)

Classification of types of analysis, role and importance of analytical chemistry in various aspects of life.

# b. Steps in a typical quantitative analysis (10 hours)

Emphasis on sampling protocol, sample preparation, wet chemistry methods, statistical evaluation of data.

## c. Review of concepts of stoichiometry (2 hours)

Mole concept, concentrations, dilution and aliquots

## d. <u>Review of concepts of equilibria (2 hours)</u>

Types of equilibrium constants, ionic equilibria, activity and activity coefficient.

## e. Gravimetric analysis (4 hours)

General steps in gravimetric analysis; types of precipitates, solubility products, factors affecting solubility of precipitates, von Weimarn ratio, co-precipitation problems, minimization of co-precipitation problems, gravimetric calculations and applications.

# f. Volumetric analysis (10.5 hours)

Acid-base titrations, buffers, acid-base indicators, titration curves, precipitation titration methods, complexometric and redox titrations, problem solving, applications. Multimethod analysis (solving problems involving combinations of classical methods of analysis)

# g. Introduction to instrumental methods of analysis (18 hours)

- Potentiometric methods (general principles and applications), quantitation methods in direct potentiometry. Potentiometric titration methods. Applications.
- Visible Spectroscopy (general principle, Beer's Law, instrumentation, qualitative and quantitative applications).

# SUGGESTED TEXTBOOKS

Harris, D.C. (2003) *Quantitative Chemical Analysis 6<sup>th</sup> ed.*, New York. W.H. Freeman & Co. (or latest edition).

Skoog, West, Holler and Crouch. (2000) Analytical Chemistry, An Introduction 7<sup>th</sup> ed., Saunders College Publishing, New York (or latest edition).

Skoog, West, Holler and Crouch. (2003) Fundamentals of Analytical Chemistry, 8<sup>th</sup> ed., Brooks Cole (or latest edition).

Harvey, D. (2000) Modern Analytical Chemistry, McGraw-Hill, USA.

Rubinson and Rubinson. (1998) Contemporary Chemical Analysis, Prentice -Hall, NJ.

Christian, G. (2003) Analytical Chemistry, 6th ed., John Wiley& Sons (or latest edition).

# SUGGESTED REFERENCES

Harris, D.C. (2004) Exploring Chemical Analysis 3rd ed., W. H. Freeman.

Skoog, D.A, Holler, F.J. and Nieman, T.A. (1997) Principles of Instrumental Analysis, 5th ed., Brooks/Cole.

AOAC on CD-ROM and EURACHEM handbook Current analytical chemistry journals

# OTHER REQUIREMENTS/EQUIPMENT

- a. Computer aided instruction software packages, such as Mathcad and Excel.
- b. Up-to-date laboratory facilities and equipment.

# 15.3.2 Analytical Chemistry 2: Instrumental Methods of Chemical Analysis

## **COURSE DESCRIPTION**

This lecture course is designed to develop knowledge and skills for analytical separations and instrumental methods of analysis. Emphasis shall be placed on the principles of instrumentation, instrument components, the limitations of measurements, and the selection of appropriate techniques for specific analytical problems.

## NUMBER OF UNITS: 3 units

**PREREQUISITES:** Analytical Chemistry 1 Lecture and Laboratory; Organic Chemistry 1 Lecture and Laboratory

# **COURSE COMPETENCIES**

At the end of the course the student should be able to:

- a. Identify a variety of analytical separations and instrumental techniques available for chemical analysis;
- b. Understand the theoretical basis for each technique.
- c. Develop critical thinking skills in the use of scientific theories to solve real world chemical problems; and
- d. Develop an appropriate analytical method for a specific problem.

# **COURSE TOPIC**

# a. Introduction to Quality Assurance (6 hours)

Quality control, quality assessment, laboratory accreditation. Traceability, reference materials, method development and validation, standard organizations and their requirements and introduction to chemometrics.

# b. Analytical separations (7 hours)

General principles, calculations and applications of preliminary separation methods such as solvent extractions, ion-exchange, complex formation, precipitation, electrodeposition, solid phase extraction.

# c. Instrumental methods of analysis:

Principles and theories, basic components, applications, characteristics of the method (figures of merit).

- Chromatographic methods (7 hours). GC, HPLC and SFC.
- Mass spectrometry (3 hours). (as detectors in GC and ICP)
- Molecular spectroscopy (7 hours) (UV-vis and Luminescence methods)
- Atomic spectroscopy (6 hours)
- Electroanalytical methods (3 hours)

## d. Others

- Radioanalytical and thermoanalytical methods (1.5 hours)
- Automated analysis. (1.5 hours)
- Methods of compositional analysis (3 hours)

## SUGGESTED TEXTBOOKS

Same as in Analytical Chemistry 1 lecture.

# 15.3.3 ANALYTICAL CHEMISTRY 1 LABORATORY

## **COURSE DESCRIPTION**

This laboratory course is designed to enable the students to master the basic skills required to perform chemical analysis based on absolute and simple instrumental methods.

## NUMBER OF UNITS: 2 units

**COREQUISITE:** Analytical Chemistry 1 Lecture

## **COURSE COMPETENCIES**

At the end of the course, the students should be able to:

- a. Perform chemical analysis using absolute and simple instrumental methods;
- b. Gather, process, evaluate and interpret experimental data;
- c. Practice safety and waste minimization in the laboratory; and
- d. Write laboratory reports that include literature citations.

#### **RECOMMENDED LABORATORY EXPERIMENTS**

The recommended topics and corresponding experiments are shown in Table 9.

Table 9. Recommended topics and sample experiments for analytical chemistry 1	
laboratory.	

Topics	Sample Experiments	
Calibration• Calibration of volumetric apparatusStatistical Treatment of Data• Determination of weight variations iSampling• Sampling techniquesGravimetric Analysis• Gravimetric determination of nickel dimethylglyoxime		
Acid - Base Titration	<ul> <li>Moisture and phosphorus analysis in fertilizers</li> <li>Determination of acetylsalicylic acid content of aspirin tablets</li> </ul>	
Complexometric Titration	• Determination of calcium carbonate content of chalk by EDTA titration	
Redox Titration	• Assay of Vitamin C tablets using iodimetric titration	
Redox Titration	• Iodometric determination of copper	
Redox Titration	• Determination of available oxygen in manganese ore	
Chromatography	• Determination of calcium by ion-exchange chromatography	
Absorption Spectrophotometry	• Colorimetric determination of iron as 1,10 - phenanthroline complex	
Potentiometry	<ul> <li>Potentiometric determination of KHP and it acid dissociation constant</li> </ul>	

#### SUGGESTED TEXTS AND REFERENCES

Suggested Textbooks: Same as in lecture

## 15.3.4 ANALYTICAL CHEMISTRY 2 LABORATORY

#### **COURSE DESCRIPTION**

This laboratory course will provide actual practice of modern analytical chemistry. With the exposure of students to the basic techniques of analytical separation and instrumental analysis, they will acquire adequate laboratory skills in the utilization of these analytical tools in real analytical problems.

#### NUMBER OF UNITS: 2 units

# **COREQUISITE:** Analytical Chemistry 2 Lecture

## **COURSE COMPETENCIES**

At the end of the course, the students should be able to:

- a. Perform chemical analysis using modern instrumental methods;
- b. Gather, process, evaluate and interpret experimental data;
- c. Practice safety and waste minimization in the laboratory; and
- d. Write laboratory reports that include literature citations.

## **RECOMMENDED LABORATORY EXPERIMENTS**

The recommended topics and corresponding experiments are shown in Table 10.

laboratory.			
Topics	Sample Experiment		
Ion – exchange chromatography	• Determination of ion - exchange capacity		
Potentiometric analysis	Potentiometric titration of phosphoric acid		
	<ul> <li>Analysis of Fluoride in Toothpaste using</li> </ul>		
	Fluoride Ion - Selective Electrode		
Voltammetry	• Voltammetric Analysis of Pb and Cd		
Atomic absorption	<ul> <li>Analysis of Ca and Mg in Limestone</li> </ul>		
spectrophotometry	<ul> <li>Analysis of Ca in food products</li> </ul>		
Solvent extraction and spectrophotometry	Solvent Extraction of Copper Oxinate		
Gas chromatography	Gas Chromatography of Alkanes		
Liquid chromatography	<ul> <li>Liquid chromatography of analgesics</li> </ul>		
Integration of instrumental	• Waste analysis		
methods	<ul> <li>Metal analysis by AAS (total)</li> </ul>		
	<ul> <li>Metal speciation and oxidation levels</li> </ul>		
	<ul> <li>Metal recovery using appropriate techniques: e.g., precipitation, ion exchange chromatography, complexation, electrochemistry</li> </ul>		
Basic electronic experiments	• Operational Amplifiers, Digital Circuits and		
(optional)	Microprocessors		

Table 10 Recommended topics and sample experiments for analytical chemistry 2 laboratory.

## SUGGESTED TEXTS AND REFERENCES

- a. Suggested References: same as in Analytical Chemistry 2
- b. Additional Reference: Sawyer, D.T, Heineman, W.R. and Beebe, J.M. (1984) *Chemistry Experiments for Instrumental Methods*, Wiley

# 15.4 FUNDAMENTALS OF BIOCHEMISTRY

## 15.4.1 BIOCHEMISTRY LECTURE

#### **COURSE DESCRIPTION**

This course covers three major areas namely: (1) the structural chemistry of the

components of living matter and how this relates to biological function; (2) the basic chemistry of the processes involved in the flow of biological information; and (3) the principles of metabolism; the totality of chemical reactions that occur in living matter.

## NUMBER OF UNITS: 3 UNITS

**PREREQUISITES:** Organic Chemistry 2 Lecture and Laboratory; Analytical Chemistry 2 Lecture and Laboratory

## **COURSE OBJECTIVES**

- a. To provide the students with a foundation in the key concepts, structures, and processes in biochemistry.
- b. To introduce key techniques in the study of biochemistry.
- c. To apply the key concepts to examples of recent findings and developments in biochemistry, molecular biology, and biotechnology.
- d. To develop students' skills in accessing and evaluating primary sources of biochemical information (including electronic databases).

## **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Describe the chemical structures that make up the components of living matter.
- b. Describe the interactions of these components that give rise to the organized supramolecular structures, cells and multicellular tissues.
- c. Explain how living organisms extract energy from the surroundings to perpetuate life.
- d. Explain how chemical reactions are regulated inside living cells.
- e. Explain how organisms store and transmit genetic information to grow and to reproduce accurately.
- f. Apply key concepts in biochemistry to explain its practical applications in the field of agriculture, medicine, pharmacy, and allied fields.
- g. Display awareness of major issues at the forefront of biochemistry.
- h. Use computers as information and research tools in biochemistry.
- i. Access, evaluate, and use primary sources of biochemical information.

# **COURSE OUTLINE**

## a. Introduction to the cell (1 hour)

- Cell structure and function
- Compartmentalization
- Cell and tissue specialization

# b. Structure and functional groups of biomolecules (15 hours)

- Amino acids and proteins
- Carbohydrates, polysaccharides, and glycoconjugates
- Nucleotides and nucleic acids
- Lipids
- Macromolecular conformation
- Membranes
- Supramolecular assemblies
- Introduction to molecular recognition
- Introduction to techniques for analysis of biological molecules

# c. The flow of biological information (12 hours)

- Biochemical unity and introduction to evolution
- The so-called Central Dogma of molecular biology and its modifications
- Basics of gene expression and gene regulation
- Introduction to techniques for gene analysis and manipulation

# d. Biological reactions and metabolism (12 hours)

- Biological catalysts
- Introduction to enzyme kinetics
- Allosteric regulation
- Metabolism and regulation
- Bioenergetics

# e. Introduction to signal transduction (2 hours)

## SUGGESTED TEXTBOOKS

Nelson, D.L. and Cox, M.M. (2004) Lehninger Principles of Biochemistry, 4<sup>th</sup> ed., W.H. Freeman (or latest edition).

- Voet, D. and Voet, J.G. (2004) *Biochemistry*, 3<sup>rd</sup> ed., John Wiley and Sons (or latest edition).
- Berg, J.M. Tymoczko, J.L. and Stryer, L. (2002) *Biochemistry, 5<sup>th</sup> ed.*, W.H. Freeman (or latest edition).

Mathews, C.K. van Holde, K.E and Ahern, K.G. (1999) *Biochemistry, 3rd ed.*, Benjamin Cummings (or latest edition).

## SUGGESTED REFERENCES

Alberts, B., Johnson, A., Lewis, J., Raff, M. Roberts, K., and Walter, P. (2002) Molecular Biology of the Cell, 4<sup>th</sup> ed., Garland.

- Lodish, H., Scott, M.P., Matsudaira, P., Darnell, J., Zipursky, L., Kaiser, C.A., Berk, Arnold., and Krieger, M. (2003) *Molecular Cell Biology*, 5<sup>th</sup> ed. W.H. Freeman (or latest edition).
- Campbell, M.K. and Farrell, S.O. (2005) *Biochemistry (with Biochemistry Now)*, 5<sup>th</sup> ed., Brooks Cole (or latest edition).

The National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health USA <u>www.pubmed.org</u> or <u>www.ncbi.nlm.nib.gov</u>

## 15.4.2 BIOCHEMISTRY LABORATORY

## **COURSE DESCRIPTION**

This laboratory course will introduce the students to common skills and techniques needed to perform biochemical investigations. It aims to provide a guide to the students in correlating certain principles of biochemistry with experimental facts.

## NUMBER OF UNITS: 2 UNITS

**COREQUISITE:** Biochemistry Lecture

## **COURSE COMPETENCIES**

At the end of the laboratory course, the students should be able to:

- a. Isolate and characterize biomolecules such as carbohydrates, proteins, lipids and nucleics acids;
- b. Analyze simple biochemical compounds; and
- c. Practice safety precautions in the laboratory.

#### **Recommended laboratory topics and sample experiments**

The recommended topics and sample experiments are presented in Table 11.

Table 11 Recommended laboratory topics and sample experiments for biochemistry laboratory.

	Topics	Experiments	Hours
1	Proteins	Isolation of proteins from plant, animal, or	9
		microbial sources	
		Column chromatography of proteins (size	
		exclusion or ion exchange)	
		Recommended: gel electrophoresis of proteins	
2	Enzymes	Effect of pH, T, activators & inhibitors	6
		Kinetics	
3	Carbohydrates	Isolation of carbohydrates from plant, animal,	9
		or microbial sources	
		Colorimetric measurement of sugars	
		Chromatographic analysis and separation of	
		sugars	
4	Lipids	Characterization of fats & oils, saponification,	9
		iodine number, free fatty acids, etc.	
		Preparation and analysis of fatty acid methyl	
		esters by GC	
		Isolation & characterization of complex lipids,	
		color reactions, thin layer chromatography	
5	Nucleic acids	Extraction and purification of DNA from	9
		animal, plant, yeast, or microbial sources	
		Quantitation of DNA by UV	
		Recommended: electrophoresis of DNA	
6	Bioinformatics	PubMed and the biochemical literature	3
		Introduction to key examples of gene, protein,	
		metabolite databases	
		Viewing 3-D structures of biomolecules	

#### SUGGESTED TEXTS AND REFERENCES

Recommended Laboratory Manual:

Bernas, G., Ysrael, M., & Bernaldez, A. (1994) Basic Laboratory Studies in Biochemistry, 3rd ed., UST Printing Office.

Boyer, R.F. (1986) Modern Experimental Biochemistry. Addison-Wesley Publishing Company Dryer, R.L. and Lata, G.F. (1989) Experimental Biochemistry. Oxford University Press, Inc., Sambrook, J. and Russell, D.W. (2001) Molecular Cloning, 3rd ed., Cold Spring Harbor Laboratory Press (or latest edition). Companion site at www.MolecularCloning.com

Others:

- Laboratory manual(s) developed for the course(s).
- MIT Open courseware: http://ocw.mit.edu/Ocw
- Biochemistry and Molecular Biology Education (BAMBED, *www.bambed,org*)
- A good resource for molecular cloning experiments for the classroom is the Biotechnology Explorer Series of Bio-Rad www.bio-rad.com, look for the Life Science Education link. While the kits are designed for high school and introductory college level, some of the material can be adapted for use by chemistry majors.
- For the computer lab sessions in biochemistry, www.proteinexplorer.org, developed by Eric Martz and coworkers, is a good starting point for macromolecular structure viewing.
- For the computer lab sessions, other key resources are the National Center for Biotechnology Information (*www.pubmed.org* or *www.ncbi.nlm.nih.gov*), the Swiss Bioinformatics Institute (*www.expasy.org*), and many others. For additional computer lab sessions, the Howard Hughes Medical Institute (*www.hhmi.org*) has a number of excellent lab animations.

## 15.5 FUNDAMENTALS OF INORGANIC CHEMISTRY

#### **COURSE DESCRIPTION**

This course focuses on the principles and trends in the chemistry of the elements and on the essentials of structure, bonding, and reactivity of inorganic systems.

NUMBER OF UNITS: 3 units

#### REQUISITES

Prerequisite: Physical Chemistry 1 Lecture and Laboratory Corequisite: Physical Chemistry 3

#### **COURSE OBJECTIVES**

This course shall provide deeper understanding of the theories and principles of bonding and structure of inorganic systems and integrate these into various technological applications. Specifically, this course seeks:

- a. To build on the principles of basic inorganic chemistry which were encountered in earlier courses, such as atomic structure and bonding, thermodynamics, and kinetics;
- b. To establish structure and reactivity correlations in inorganic systems;
- c. To introduce the concepts of symmetry and group theory and their application in understanding molecular behavior and structure;
- d. To introduce the descriptive chemistry of representative elements and transition elements and their chemical compounds;
- e. To provide insight into the many applications of the concepts of inorganic chemistry in areas such as agriculture, molecular biology, medicine, and materials;
- f. To gain enhanced independence in scholarship through active learning exercises; and
- g. To report new discoveries in the field of inorganic chemistry.

#### **COURSE COMPETENCIES**

By the end of the course, the student should be able to:

- a. Acquire an in-depth knowledge of a range of topics in advanced inorganic chemistry;
- b. Critically evaluate articles published concerning inorganic chemistry; and
- c. Formulate sound opinions in subject areas at the forefront of inorganic chemistry and where controversies may still exist.

# COURSE OUTLINE

- a. Basic Inorganic Principles
- Atomic Structure (3 hours)

   Principles of Quantum Mechanics
   Quantum Numbers
   Effective nuclear charge, Slater's orbitals
   Periodic Properties of Atoms
- Molecular Structure (3 hours)
   o Valence Bond Theory
   o Molecular Orbital Theory
- Molecular Shape and Symmetry (4.5 hours)
   Symmetry analysis and group theory
   Applications of group theory to molecular structure and bonding
- Reactivity of Inorganic Compounds (6 hours)
  - Acids and Bases (major acid-base concepts; systematics of Lewis acids and bases; hard and soft acids and bases)
  - Redox Chemistry (redox stability in water; diagrammatic presentation of potential data)
- b. Coordination Chemistry (7.5 hours)
- Structure, Geometry and Isomerism
- Bonding theories of coordination compounds
- Reactions and Mechanisms
- c. Inorganic Spectroscopy (4.5 hours)
- Electronic Spectroscopy of free ion states
- Electronic spectra of complexes
- Bonding and spectra of simple metal clusters
- Vibrational spectroscopy
- d. Solids and Materials Chemistry (4.5 hours)
- Crystal Structures
- Thermodynamic aspects
- MO theory of solids and band structure
- Superconductivity
- Bonding in Ionic Solids
- e. Systematic Chemistry of Main Group Elements (4.5 hours)
- Physical properties
- Reactivities of the elements and their compounds
- f. Organometallic Chemistry (4.5 hours)
- 18-electron rule
- M-C bonding in organometallic compounds
- Reactions and mechanisms
- g. Special Topics in Inorganic Chemistry (6 hours)
- Catalysis and important industrial processes
- Bioinorganic chemistry
- Inorganic materials
- Environmental and atmospheric chemistry

# SUGGESTED TEXTBOOKS

Meissler and Tarr. (2002) Inorganic Chemistry, 3rd ed. McGraw Hill.

Housecroft, C.E. and Sharpe, A.G. (2005) Inorganic Chemistry, 2nd ed. Prentice Hall.

- Shriver, D.F., Atkins, P.W., and Langford, C.H. (1999) *Inorganic Chemistry, 3rd ed.* Oxford University Press.
- Huheey, J.E., Keiter, E.A. and Keiter, R.L. (1993) Inorganic Chemistry: Principles of Structure and Reactivity 4th ed. Harper and Row (or latest edition).
- Douglas, McDaniel, and Alexander. (1994) Concepts and Models in Inorganic Chemistry, 3rd ed. Wiley.

Cotton, Wilkinson and Gaus. (2002) Basic Inorganic Chemistry, 3rd ed. Wiley.

#### SUGGESTED REFERENCES

Various journals in Inorganic Chemistry

## 15.5.1 INORGANIC CHEMISTRY LABORATORY (OPTIONAL)

#### **COURSE DESCRIPTION**

The laboratory should complement the lecture portion. Each exercise should involve synthesis as one part, and analysis or characterization of the product as the second part.

#### NUMBER OF UNITS: 1 unit

## **COREQUISITE:**

Inorganic Chemistry Lecture

## **COURSE COMPETENCIES**

At the end of the laboratory course, the students should be able to:

- a. Synthesize, purify and characterize inorganic compounds such as bioinorganic complexes, coordination compounds and solid state materials; and
- b. Practice safety precautions in the laboratory.

#### RECOMMENDED LABORATORY TOPICS AND SAMPLE EXPERIMENTS

The recommended topics and sample experiments are presented in Table 12.

	Topics	Suggested Experiments
1	Bioinorganic complexes	For example: Amino acid complexes, metal complexes used for DNA cleavage, oxygen uptake of a cobalt complex, haemoglobin, cytochrome oxidases, etc.
2	Coordination compounds	For example: $[Co(NH_3)_4CO_3]NO_3$ and $[Co(NH_3)_5)Cl]Cl_2$ ; optical resolution of $Co(en)_3^{+3}$ etc.
3	Compounds of the main-group elements	For example: Tin-containing compounds, Main Group Chemistry: Boron and Silicon, etc
4	Solid-state compounds	For example: Preparation and characterization of some semiconductors: Preparation of a superconductor, etc
		some semiconductors: Preparation of a

Table 12. List of inorganic chemistry laboratory topics and experiments.

#### SUGGESTED TEXTS AND REFERENCES

Laboratory manual(s) developed for the course(s).

MIT Open courseware: *http://ocw.mit.edu/Ocw* 

- Tanaka, J. and S.L. Suib. (1999) *Experimental Methods in Inorganic Chemistry*. Upper Saddle River: Prentice Hall.
- Girolami, G.S., Rauchfuss, T.B. and Angelici, R.J. (1999) Synthesis and Techniques in Inorganic Chemistry. 3rd ed. Sausalito: University Science Books.
- Szafran, Z., Pike, R.M., and Singh, M.M. (1991) Microscale Inorganic Chemistry: A Comprehensive Laboratory Experience

Pass, G., Sutcliffe, H. (1982) Practical Inorganic Chemistry.

Jolly, W.L. (1970) The Synthesis and Characterization of Inorganic Compounds.

Inorganic Chemistry (Publisher: American Chemical Society)

Organometallics (Publisher: American Chemical Society)

# 15.6 PHYSICAL CHEMISTRY

#### **OVERVIEW OF SUBJECT AREA**

The aim of the Physical Chemistry series is to introduce the fundamental concepts and general principles applied to the understanding of the behavior of matter.

The series will introduce the theoretical and experimental approaches to the study of the physical properties of chemical systems and their reactions at the macroscopic and atomic/molecular levels. The series will also develop problem solving skills of students in the major areas of Physical Chemistry

The scope of the Physical Chemistry series includes the following core topics:

- a. Chemical thermodynamics
- b. Dynamics: physical and chemical kinetics
- c. Quantum chemistry
- d. Statistical thermodynamics

The courses incorporate the following application of the theories in the core areas:

- a. Electrochemistry
- b. Surface Chemistry, Macromolecules and Colloids
- c. Spectroscopy electronic, rotation and vibration and laser spectroscopy
- d. Other topics: solid-state chemistry/materials chemistry, photochemistry/atmospheric chemistry.

## **COURSE OBJECTIVES**

At the end of the physical chemistry series, students should be able to:

- a. Understand the physico-chemical properties of macroscopic systems and their transformations through the principles that govern their equilibrium properties;
- b. Gain insight into the behavior of chemical systems at the atomic and molecular levels;
- c. Understand the assumptions of the various models used to describe chemical systems so students will learn to apply them critically;
- d. Perform calculations dealing with important physico-chemical phenomena;
- e. Acquire experience on modern experimental techniques in Physical Chemistry;

- f. Learn methods of data collection including computer interfacing and methods for assessing validity of measurements, estimating errors and relating data to models for the systems under study; and
- g. Acquire the ability to decide on appropriate physico-chemical techniques in solving chemical problems.

## 15.6.1 Physical Chemistry 1: Chemical Thermodynamics

## **COURSE DESCRIPTION**

This course provides the foundations in chemical thermodynamics, physical and chemical equilibria, and an introduction to statistical thermodynamics.

## **NUMBER OF UNITS:** 3 units

**PREREQUISITES:** Organic Chemistry 1 Lecture and Laboratory; Analytical Chemistry 1 Lecture and Laboratory; Integral Calculus

# **COURSE COMPETENCIES**

At the end of the course, the students must be able to:

- a. Apply the models for ideal and real gases to chemical problems.
- b. Apply the laws of thermodynamics to physical and chemical processes.
- c. Construct and interpret phase diagrams for substances and mixtures.
- d. Understand the derivation of equilibrium properties of macroscopic systems from microscopic properties.

## **COURSE OUTLINE**

- a. Ideal and real gases and equations of state; related math methods (6 hours).
- b. Nature of thermodynamics; formalism; systems, boundaries, states, processes related math concepts (3 hours)
- c. Internal energy and enthalpy; heat, work, First Law of Thermodynamics applied to different processes; related math concepts; standard functions; thermochemistry; calorimetry (12 hours)
- d. Second and Third Laws of Thermodynamics; Entropy, Gibbs Energy, calculation of changes in thermodynamic functions; standard functions; Maxwell relations and Gibb's Duhem equation (12 hours)
- e. Phase equilibria; Clausius-Clapeyron for substances; binary and multicomponent phase equilibria of ideal solutions; colligative properties of ideal dilute solutions (9 hours)
- f. Introduction to Statistical Mechanics (3 hours)

# SUGGESTED TEXTBOOKS (PHYSICAL CHEMISTRY 1 AND 2)

- a. Atkins, P.W. and de Paula, J. (2002) Physical Chemistry, 7th ed. Oxford University Press.
- b. Ball, D. W. (2003) Physical Chemistry, Brooks/Cole.
- c. Laidler, K.J., Meiser, J. H. and Sanctuary, B.C. (2003) *Physical Chemistry*, 4<sup>th</sup> ed., Boston: Houghton Mifflin Co.
- d. Levine, I. N. (2001) Physical Chemistry, 5th ed., McGraw-Hill, New York.
- e. McQuarrie, D.A. and Simon, J.D. (1997) *Physical Chemistry, A Molecular Approach,* University Science Books.
- f. Mortimer, R.G. (1993) Physical Chemistry, Benjamin Cummings.

g. Silbey, R. J., Alberty, R.A., and Bawendi, M. (2005) *Physical Chemistry, 4th ed.*, John Wiley and Sons Inc.

#### SUGGESTED REFERENCES

- a. Callen, H. (1985) Thermodynamics 2nd ed., J. Wiley and Sons.
- b. Klotz, I. and Rosenberg.M. (2000) *Chemical Thermodynamics: Basic Theory and Methods* 6th ed., Wiley-Interscience.

#### **OTHER REQUIREMENTS**

Computers and mathematical software: Mathcad, Mathlab, Mathematica, Excel, or equivalent software; multimedia materials, AV equipment

#### 15.6.2 Physical Chemistry 2: Thermodynamics and Kinetics

#### **COURSE DESCRIPTION**

This course is a continuation of Physical Chemistry 1. This course will discuss the following topics: thermodynamic properties of chemical systems with emphasis on non-ideal systems; electrochemistry; transport properties; chemical kinetics; surface chemistry, macromolecules and colloids; photochemistry; solid state and other applications.

#### NUMBER OF UNITS: 3 units

**PREREQUISITE:** Physical Chemistry 1 Lecture

#### **COURSE COMPETENCIES**

At the end of the course the student must be able to:

- a. Evaluate parameters related to non-ideal behavior of gases and mixtures such as gas fugacities, activity coefficients and activities of components of mixtures.
- b. Relate the thermodynamic properties to the equilibrium constants of electrochemical cells.
- c. Relate the flow properties of atoms, molecules and ions to the bulk transport properties of gases, liquids and ions in solutions.
- d. Discuss the principles and theories of chemical kinetics including processing of kinetic data and proposing reaction mechanisms.
- e. Characterize surface phenomena in terms of equilibrium and dynamic properties.
- f. Explain the techniques for studying the structure and physical properties of other systems such as macromolecules, colloids and atmospheric photochemical reaction systems.

#### **COURSE OUTLINE**

- a. Thermodynamics; fugacities, activity, activity coefficients, partial molar properties of solutions (6 hours)
- b. Equilibrium electrochemistry (5 hours)
- c. Kinetic Molecular Theory; transport properties of gases and liquids (5 hours)
- d. Solutions of electrolytes: transport properties of ions and their applications; equilibrium properties; ionic theories; activity coefficients (4 hours)
- e. Chemical kinetics: rate laws, Arrhenius equation, mechanisms and applications to enzyme catalysis and photochemical reactions, theories of elementary reactions; techniques for fast reactions (10 hours)

- f. Surface chemistry, Macromolecules and Colloids: thermodynamic properties; surface tension measurements; adsorption isotherms; heterogeneous kinetics; size, shape and molar mass of macromolecules; properties of colloids and applications (6 hours)
- g. Special topics (9 hours)

## SUGGESTED TEXTBOOKS AND REFERENCES

Same as Physical Chemistry 1

#### **OTHER REQUIREMENTS**

Computers and mathematical software: Excel, or equivalent software; multimedia materials, AV equipment

## 15.6.3 Physical Chemistry 3: Quantum Chemistry

#### **COURSE DESCRIPTION**

This course shall cover the fundamental principles and equations of quantum chemistry and statistical thermodynamics, and their applications to atomic and molecular spectroscopy. This can be offered independent of Physical Chemistry 1 & 2 provided the student has taken Organic Chemistry 1, Analytical Chemistry 1 and Integral Calculus.

#### **NUMBER OF UNITS:** 3 units

**PREREQUISITES:** Organic Chemistry 1 Lecture and Laboratory; Analytical Chemistry 1 Lecture and Laboratory; Integral Calculus

#### **COURSE COMPETENCIES**

At the end of the course the student should be able to:

- a. Apply the formalism to simple systems (particle-in-a box, harmonic oscillator, rigid rotor) and relate the results to chemical systems.
- b. Determine spectroscopic states for the elements.
- c. Construct the wave functions for the many electron atoms.
- d. Solve problems in atomic and molecular spectroscopy.
- e. Apply the fundamental concepts of statistical thermodynamics to simple systems.

#### **COURSE OUTLINE**

- a. Background of Quantum Mechanics; formalism of Quantum Mechanics (6 hours)
- b. Operators, eigenvalue problems, postulates and application to simple systems (6 hours)
- c. Exactly soluble problems in one, two and three dimensions (9 hours)
- d. Approximate methods and application to atoms and molecules; related math methods (9 hours)
- e. Vibrational and rotational spectroscopy (4 hours)
- f. Statistical Thermodynamics: canonical ensembles and partition functions; application of results of quantum chemistry to calculate thermodynamic quantities (9 hours)

#### SUGGESTED TEXTBOOKS

Same as Physical Chemistry 1

# SUGGESTED REFERENCES (IN ADDITION TO THE REFERENCES FOR PHYSICAL CHEMISTRY 1 AND 2)

- a. Atkins, P.W. (1983) Molecular Quantum Mechanics, Oxford University Press.
- b. Levine, I.N. (2000) Quantum Chemistry, Prentice-Hall.
- c. Lowe, J.P. (1993) Quantum Chemistry, Academic Press.
- d. McQuarrie, D.A. (2000) Statistical Mechanics 2nd rev. ed., University Science Books.
- e. McQuarrie, D.A. (1983) Quantum Chemistry, University Science Books.
- f. Pauling, L. and Wilson, E.B. (1935) Introduction to Quantum Mechanics with Applications to Chemistry, McGraw-Hill, (reprinted by Dover Publications, 1985).
- g. Wieder, S. (1973) The Foundations of Quantum Theory, Academic Press.

# OTHER REQUIREMENTS (IN ADDITION TO THOSE LISTED FOR PHYSICAL CHEMISTRY 1 AND 2)

Computers and recommended software/language for programming and modeling: Fortran, Hyperchem, Alchemy, MOPAC, Moby, Spartan & others.

# 15.6.4 PHYSICAL CHEMISTRY LABORATORY 1 and 2

#### **COURSE DESCRIPTION**

The laboratory courses demonstrate the techniques for evaluating physical properties of chemical systems described in the accompanying lecture.

#### NUMBER OF UNITS

Physical Chemistry 1 Laboratory: 1 unit Physical Chemistry 2 Laboratory: 1 unit

#### REQUISITES

<u>Physical Chemistry 1 Laboratory</u> Corequisite: Physical Chemistry 1 Lecture

Physical Chemistry 2 Laboratory

Prerequisite:Physical Chemistry 1 Lecture and LaboratoryCorequisite:Physical Chemistry 2 Lecture

## **COURSE COMPETENCIES**

At the end of the physical chemistry laboratory courses, the student should be able to:

- a. Apply physical methods in characterizing systems at equilibrium;
- b. Apply physical methods to kinetic problems;
- c. Evaluate physical properties of non-ideal systems; and
- d. Relate experimental results to models for chemical systems

## COURSE OUTLINE

The recommended topics and sample experiments are presented in Table 13.

Topic	Sample Experiment
Ideal Gas	• Gas density and MW
	• Viscosity of gases
	• Thermal conductivity of
D 10	• Gases
Real Gases	• Joule Thomson coefficient of gases
Thermochemistry	<ul> <li>Enthalpy of combustion of substances</li> </ul>
	• Heats of solution
Phase Equilibria	
1 component system	Vapor pressure of a liquid
2 component system	Liquid-Solid Equilibrium
r	Liquid-Vapor Equilibirum
3 component system Solutions	• Ternary System
Partial Molar Properties	Partial Molal Volume
	<ul> <li>Partial Molar Enthalpy of Mixing</li> </ul>
Colligative Properties	<ul> <li>Freezing point depression</li> </ul>
	<ul> <li>Boiling Freezing point elevation</li> </ul>
Electrochemistry	• Determination of activity and activity coefficients from cell emf
	<ul> <li>Electrochemical cells with liquid junctions</li> </ul>
Transport Properties and Applications	•
Macromolecules	• MW of polymers from viscosity of solutions
Ions in Solutions	<ul> <li>Constant of Ionization from Conductivity Measurements</li> </ul>
	• Transference Numbers by Hittorf Method
Chemical Kinetics	
Rate Law: Order of	• Saponification of ethyl acetate by conductivity
Reaction	measurements
Temperature Effects	• Inversion of sucrose
Surface Properties	• Surface tension of solutions
	Adsorption isotherms
Spectroscopy and Molecular Structure	
Electronic Spectroscopy	• UV-VIS spectrum of a conjugated dye

Table 13. List of topics and sample experiments for physical chemistry laboratory 1 and 2. (At least one experiment from each topic listed below must be done. Other applied physical chemistry areas are also recommended.)

Table 13 continued	
Topic	Sample Experiment
Vibrational and Rotational Spectroscopy	• Infrared spectrum spectrum of HCl
Molecular modeling/computer based exercises	<ul> <li>Molecular modeling; curve fitting methods; root seeking methods;</li> </ul>

## Suggested Texts and references (Laboratory Manuals)

- a. Halpern, A. M. and Reeves, J. H. (1998) *Experimental Physical Chemistry: A Laboratory Textbook,* Scott, Foresman and Co.
- b. Hehre, W.J., Yu, J., Klunzinger, P.E., and Lou, L. (1998) *A Brief Guide to Molecular Mechanics and Quantum Chemical Calculations.*
- c. Hori, K. and Yamazaki, S. (1998) Computational Chemistry Experiments.
- d. Laboratory manual(s) developed for the course(s).
- e. MIT Open courseware: http://ocw.mit.edu/Ocw
- f. Schoemaker, D.P. Garland, C.W. and Nibler, J.W. (1989) *Experiments in Physical Chemistry, 5th ed.*, Mc-Graw Hill (or latest edition).
- g. Bettelheim, F.A. (1971) Experimental Physical Chemistry, W.B. Saunders.
- h. Sime, R.J., (1990) *Physical Chemistry: Methods, Techniques and Experiments*, Saunders College Publications (or latest edition).

#### EQUIPMENT

- a. Glassware which may be fabricated: Dumas bulb or long neck Florence flask, closed tube Hg manometer, gas viscometer; capillary for surface tension
- b. Thermal conductivity cell
- c. Conductivity Bridge/cell
- d. Electrodes: glass and calomel
- e. pH meter
- f. Dewar flask
- g. Bomb calorimeter
- h. Pycnometer
- i. Viscometer
- j. Surface tension apparatus: tensiometer
- k. Vacuum pump
- l. Boiling point apparatus
- m. UV-vis spectrophotometer (scanning)
- n. FT IR spectrophotometer (with gas cell)
- o. Abbe refractometer
- p. Polarimeter
- q. Contact angle goniometer
- r. Analytical balances
- s. Software for PC
- t. Hittorf Moving Boundary Apparatus

# NOTES ON THE RECOMMENDATIONS FOR PHYSICAL CHEMISTRY LECTURE AND LABORATORY

- a. If the instructor feels that there is not enough time to cover the topics during the lecture session, it is suggested that some of the topics be discussed during the laboratory session. Examples of these would be topics in molecular spectroscopy, electrochemistry, interfacial phenomena, and kinetics. These topics need not take up a large chunk of the lecture time, but in-depth quantitative (computational) treatment may be incorporated in the laboratory experiments, as usually is the case, anyway. Thus, this will free up lecture time that can be devoted to other topics.
- b. A lot of time in the lecture is often taken up by mathematical computations because of the poor background of the students in differential and integral calculus. This may be alleviated by directly collaborating with the Math department so that similar problems might be introduced in the Math courses.
- c. Coverage of Electrochemistry should be coordinated with the General and Analytical Chemistry courses to improve continuity and minimize overlap. It is suggested that Electrochemistry be included as an integral part of the Physical Chemistry curriculum because most economically feasible Physical Chemistry experiments involve electrochemical apparatus.
- d. Many schools offer Spectroscopy as a separate course and it is often covered as part of Organic and Analytical Chemistry. Analytical Chemistry discusses spectroscopy as part of instrumentation (different spectrometers, etc.) and quantitative measurement (Beer-Lambert's Law-type of discussions). Organic Chemistry, on the other hand, discusses spectroscopy as applied to elucidation of organic chemical structures (UV-Vis, NMR, IR, Mass Spectrometry, etc.), the treatment of spectroscopy in Physical Chemistry should focus on its quantum mechanical bases. For example, the Beer-Lambert law in Physical Chemistry should be discussed in terms of the coupling of the dipole transition moment and the electric field component of light; or the broadening of the NMR or IR bands can be explained as resulting from the inherent Heisenberg uncertainty principle, overlapping of low energy transitions, etc. It is also a good time to recapitulate the interdependencies of the traditional divisions of chemistry.
- e. The Physical Chemistry teacher should be given the freedom to develop the sequence of the topics as long as the essential topics are covered.
- f. In the recommendations for the laboratory section, the experiment titles are given only as suggestions for a given topic. Other experiments may be substituted.
- g. Examples of PC-based software for Computer Modeling Exercises in the lab include HyperChem, Alchemy, MOPAC, and Moby; each includes a routine for energy minimization plus a variety of viewing options (e.g., stereo images) options. Phy Chem calculations and graphing may be done using any of the following: MathCAD, MathLAB, Mathematica, Excel, and others.

## 15.7 THESIS AND PROFESSIONAL EXPOSURE

#### INTRODUCTION

These courses will provide students with the opportunity to apply their knowledge and skills in solving research (thesis) and real-world problems (professional exposure). Institutions have the following options:

- a. Thesis (6 units); or
- b. Combination of thesis and professional exposure (6 units total)

NUMBER OF UNITS: 6 units in total

**PREREQUISITES:** Student must be of senior standing.

## 15.7.1 THESIS

#### **O**VERVIEW

Undergraduate research is an indispensable part of a world-class undergraduate degree program in chemistry. This course description is benchmarked against the current American Chemical Society (ACS) guidelines for the conduct of undergraduate thesis research. The ACS Committee on Professional Training strongly encourages making research available to undergraduates as an advanced course option because it "unifies and extends the ACS-approved core chemistry curriculum". It develops traits in the student that will result in personal and professional growth. At the same time, it requires the faculty to remain up-to-date in his/her field, leading to increased enthusiasm, better morale and improved teaching. An active research program is also a means of attracting external funding and attracting and keeping talented faculty.

#### **COURSE DESCRIPTION**

Independent active research to be conducted under the guidance of a senior faculty adviser or mentor; the topic may be basic, applied or theoretical in nature.

#### NUMBER OF UNITS

Undergraduate Thesis 1: 3 units Undergraduate Thesis 2: 3 units

**PREREQUISITE:** Advanced Chemistry Laboratory series; This is a 4th year level course and the student must have completed <u>most</u> of the core Chemistry courses.

#### **COURSE OBJECTIVES**

This course aims to train the student to do independent research in chemistry, and to be able to present the work in a seminar.

#### **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Demonstrate problem-solving skills by applying classroom knowledge and laboratory skills in a research environment;
- b. Gather and critically assess relevant literature;
- c. Design experiments to test a scientific hypothesis and to make observations where the outcome is unknown;
- d. Interpret results and draw conclusions from the experiments or calculations;
- e. Use and care for equipment;
- f. Demonstrate a spirit of open inquiry, persistence and creativity and a strong work ethic;
- g. Work independently but also as a part of a team with a supervisor;
- h. Develop technical writing skills not only in the preparation of the laboratory notebook and progress reports for the mentor;
- i. Communicate effectively through well-written research reports and oral presentations; and
- j. Practice ethical principles in the conduct of scientific research.

#### SUGGESTED TEXTBOOKS AND REFERENCES

- a. Kanare, H.M. (1985) Writing the Laboratory Notebook, American Chemical Society, Washington, DC.
- b. Dodd, J. S. (Ed) (1997) The ACS Style Guide, American Chemical Society, Washington, DC.
- c. Cain, B. E. (1988) *The Basics of Technical Communicating*, ACS Professional Reference Book American Chemical Society, Washington, DC.
- d. There are a number of references which are available on ethics. Some examples include: Chemist's Code of Conduct (American Chemical Society, *http://www.chemistry.org*), and Ethics in Science (Prof. H. Bauer, *http://www.chem.vt.edu*).

## **COMMENTS**

This course assumes the availability of instrumentation, facilities, chemicals, and other materials needed for research.

#### RECOMMENDATIONS

- a. Regular supervision by, and consultations with the adviser are essential. The adviser should pay careful attention to the conduct of the experiments or calculations and the interpretation of results.
- b. The supervisor should carefully evaluate data quality, progress reports and thesis manuscripts. The output can be presented in conferences, and if appropriate, publication in a peer-reviewed journal.
- c. The adviser should emphasize and practice research ethics.
- d. The university should have an intellectual property (IP) policy which covers patentable inventions, devices, etc. The IP rights of the student and faculty adviser should be protected.

## **E** 15.7.2 PROFESSIONAL EXPOSURE

## **OVERVIEW**

This will enable the student to obtain experience in the practice of chemistry in various settings such as private, government, industry and academe laboratories, and research institutions.

Through this experience, students will acquire additional skills and insights on the application of chemistry in solving real-world problems. It will also strengthen the link between the study and practice of chemistry.

# ARTICLE VII GENERAL REQUIREMENTS

## **SECTION 17 Program Administration**

## 17.1 Composition

The B.S Chemistry Program shall be administered by a/under a Chemistry department or institute headed by its own chair or director and having its own set of full-time faculty.

# 17.2 Dean or Department chair

A Higher Education Institution (HEI) offering a science program shall have a full-time Dean or Department Chair.

# a. Dean

The dean of the college administering the BS Chemistry program must possess a master's degree in a discipline offered within the college.

## b. Department chair

The head of the Chemistry department or institute offering a BS Chemistry program must at least be a MS Chemistry degree (with thesis) holder or allied fields (with thesis) and a registered chemist.

# 17.3 Monitoring of the BS Chemistry program

The CHED may, at any time, review the BS Chemistry program. For this purpose, the HEI should keep a complete faculty and student file. For faculty, this shall include their faculty load, teaching, research and outreach activities, evaluation, and other relevant information. For students, this shall include courses, theses, projects, examinations, and other relevant information.

# Section 18 Faculty

# 18.1 Qualifications of faculty

All faculty teaching in the BS Chemistry program must have the minimum of a MS degree in chemistry or any allied field cited in Section 6.

All faculty members handling chemistry courses required for the licensure examination for chemists must be a registered chemist.

## 18.2 Full time faculty members

- a. At least 50% of the teaching staff in the BS Chemistry program must be full-time faculty members.
- b. At least 60% of the full-time faculty must have graduate degrees in chemistry. At least one of the full-time faculty must have an earned Ph.D. degree in chemistry and at least two with an MS degree (with [JC2]thesis) as their highest degree.
- c. Faculty with only undergraduate degrees must be actively pursuing graduate degrees in chemistry.

# 18.3 Teaching Load

Teaching load requirements for BS Chemistry shall be as follows:

- a. Full time faculty members should not be assigned more than four (4) different courses/subjects within a semester.
- b. In no instance should the aggregate teaching load of a faculty member exceed 30 units per semester (inclusive of overload and teaching loads in other schools).
- c. Teaching hours per day should not exceed the equivalent of 6 lecture hours.

# 18.4 Faculty academic load

The regular fulltime load of a chemistry faculty member shall be defined as the total

academic load, which is an aggregation or combination of teaching, research and administration

The regular academic load of PhD/MS Faculty should include research and/or development projects and outreach.

The allotment of a research load to the faculty with corresponding compensation is highly encouraged.

Only faculty members with graduate degrees by research should be assigned as thesis advisers.

# 18.5 Faculty development

The institution must have a system of staff development. It should encourage the faculty to:

- a. Pursue graduate studies or post-graduate training;
- b. Undertake research activities and to publish their research output;
- c. Give lectures and present papers in national/international conferences, symposia and seminars;
- d. Attend seminars, symposia and conferences for continuing education; and
- e. Be active members of recognized professional associations.

The institution must provide opportunities and incentives such as:

- a. Tuition subsidy for graduate studies;
- b. Study leave with pay;
- c. Deloading to finish a thesis or carry out research activities;
- d. Travel grants which could include conference registration, accommodation and transportation for academic development activities such as special skills training and attendance in national/ international conferences, symposia and seminars; and
- e. Awards & recognition.

## Section 19 Instructional Standards

HEIs shall at all times maintain a high standard of instruction through:

- a. Periodic evaluation (including teaching competence, research capabilities, scholarly outputs, dedication to work and integrity) of the teachers by students, peers and the chairman of the department;
- b. Provision and maintenance of adequate laboratory facilities;
- c. Provision of at least one laboratory instructor for every 25 students;
- d. Keeping the number of students in a regular lecture class to not more than forty (40) except when provisions are made for a larger class;
- e. Adoption of textbooks and other instructional materials that are up to date (ideally not older than 5 years) in content and not violative of Philippine laws;
- f. Use of modern techniques and technology for improving teaching and learning quality;
- g. Periodic evaluation of the chemistry curriculum at least every 5 years;
- h. Definite and valid system of evaluating student class performance; and
- i. System of awards and recognition for outstanding faculty and student performance.

# Section 20 Library

# 20.1 Policy

Libraries service the instructional and research needs of the staff and students making it one of the most important service units within an HEI. It is for this reason that libraries should be given special attention by HEI administrators by maintaining it with a wide and up-to-date collection, qualified staff, and communications and connectivity portals.

# 20.2 Library staff

The Head Librarian should: 1) have an appropriate professional training; 2) be a registered librarian; and 3) have a Master's degree.

The library should be: 1) staff with one full time professional librarian for every 1,000 students and 2) a ratio of 1 librarian to 2 staff / clerks should be observed.

## 20.3 Library holdings

Library holdings should conform to existing requirements for libraries. For the BS Chemistry program, the libraries must provide 5 book titles per professional course found in the curriculum at a ratio of 1 volume per 15 students enrolled in the program. These titles must have been published within the last 5 years.

The HEI is likewise encouraged to maintain periodicals and other non-print materials relevant to environmental science to aid the faculty and students in their academic work. CD-ROMs could complement a library's book collection but should otherwise not be considered as replacement for the same.

## 20.4 Internet access

Internet access is encouraged but should not be made a substitute for book holdings.

## 20.5 Space requirements

At least 126 m<sup>2</sup>. or approximately 2 classrooms shall be required for the library. It should include space for collections, shelving areas, stockroom, office space for staff and reading area

The library must be able to accommodate 5% of the total enrollment at any one time.

## 20.6 Finance

All library fees should be used exclusively for library operations and development for collections, furniture and fixtures, equipment and facilities, maintenance and staff development.

## 20.7 Networking

Libraries shall participate in inter-institutional activities and cooperative programs whereby resource sharing is encouraged.

## 20.8 Accessibility

The library should be readily accessible to all.

## 20.9 Office hours

The library should be open to serve the needs of the users.

# Section 21 Educational Technology Centers

The institution should provide facilities to allow preparation, presentation and viewing of audio-visual materials to support instruction.

# Section 22 Facilities and Equipment

# 22.1 Laboratory requirements

Laboratories should conform to existing requirements as specified by law (RA 6541, "The National Building Code of the Philippines" and Presidential Decree 856, "Code of Sanitation of the Philippines"). List of required and recommended equipment are listed in each of the course requirements above.

Adequate instrumentation and support facilities are crucial to the quality of the B.S. Chemistry program. The proper training of the Chemistry student requires that the essential equipment is available in the laboratory. Table 14 lists the support facilities required for the laboratory courses.

The following points should be emphasized:

- The Chemistry department must see to it that the condition in the laboratory considers human safety such as proper ventilation, access to emergency and first aid equipment, among others (See Appendix B).
- The list of instruments is intended for undergraduate B.S. Chemistry laboratory courses. As such, the purpose of the instruments is mainly instructional. In general, the simpler, more robust models are preferred.
- The Chemistry department must see to it that the conditions for proper operation and maintenance of the instrument are adequate, in particular: stability of electricity, protection from dust, heat and other inappropriate conditions.
- There should be faculty and/or staff who are adequately trained and knowledgeable in the principles, operation and maintenance of the equipment.
- The students should be properly trained in the principles and operation of the various equipment. Students should have reasonable access to the instruments.
- Students should be properly trained/informed about proper disposal of chemical waste.

Support facility	Comments				
1	Essential. Capacity should be sufficient to supply distilled water for all chemistry laboratories.				
Ion-exchange unit (for water purification)	Optional. Used primarily for Analytical Chemistry, Biochemistry, and Physical Chemistry				
Fume hood/ Cupboard	Essential. The laboratories used for the following courses should have fume hoods: General Chemistry, Organic Chemistry, Analytical Chemistry, Biochemistry and Inorganic Chemistry. The hood area should be sufficient to accommodate the number of students who are doing the laboratory.				

Table 14. List of support facilities for a chemistry laboratory.

# 22.2 Laboratory Staff

- a. Each department with laboratory/ies shall have full-time properly trained laboratory technician/s to maintain laboratory facilities.
- b. Each department with laboratory/ies shall assign at least one personnel as the <u>laboratory safety officer /chemical waste manager</u> available at all times to respond to emergencies such as fire, chemical accidents, first aid needs, earthquakes, and other exigencies.

# 22.3 Laboratory equipment

Table 15 lists the required instrumentation for each of the laboratory subjects. The rightmost column ("FREQ") summarizes the number of courses that requires the particular instrument and is an indication of its importance.

Table 15. List of recommended instrumentation and the frequency of their use. (Abbreviations used: Gen=General Chemistry; Org=Organic Chemistry; Ana=Analytical Chemistry; Inorg=Inorganic Chemistry; Phy=Physical Chemistry; FREQ=Frequency.)

Instrument	Gen	Org	Ana	Bio	Inorg	$\operatorname{Phy}$	FREQ
Aerator (large fish tank aerators will do)					х		1
Analyzer, Thermogravimetric					х		1
Analyzer, Thermogravi-metric			х		х	х	3
Analyzer, Voltammetric			х			х	2
Autoclave				х			1
Balance, analytical		х	х	х		х	4
Balance, analytical (0.0001 g sensitivity)					х		1
Balance, electronic	Х	х		х	х	х	5
Balance, magnetic					х	х	2
Balance, top loading		х		х			2
Barometer	Х					х	2
Beakers		х					1
Boiling point apparatus						х	1
Burner					х		1
Calorimeter						х	1
Capillary for surface tension						х	1
Calorimeter, Bomb						х	1
Cell, Conductivity Bridge						х	1
Cell, thermal conductivity cell						х	1
Centrifuge	х		х	Х			3
Chromatograph, basic gas			х				1
Chromatograph, gas		х	х	х		х	4
Chromatograph, High Performance Liquid		х	х	х		х	4
Chromatograph, thin layer plates				х			1
Chromatograph, Thin Layer Plates & Developing Tank		х					1
Closed tube Hg manometer						х	1
Colorimeter	х	х	х	х	х	х	6
Dewar flask						х	1
Dialysis bag				х			1
Dumas bulb or long neck Florence flask						х	1

Instrument	Gen	Org	Ana	Bio	Inorg	$\operatorname{Phy}$	FREQ
Electrodes: glass and calomel						x	1
Electrophoresis w/ power supply				х			1
Electrophoresis, gel				x			1
Flasks		х					1
Funnel, buchner		х					1
Funnel, separatory		х					1
Funnels		х					1
Furnace			х	х			2
Gas cylinders for nitrogen gas					х		1
Gas viscometer						х	1
Goniometer, contact angle						х	1
Ground Glass Joint Kit for Organic Chemistry		х					1
Hittorf Moving Boundary Apparatus						х	1
Hot plate					х		1
Hot Plate & Stirplate		х					1
Melting point apparatus		х			х	х	3
Meter, conductivity			х		х	х	3
Meter, pH	х	х	x	х	X	х	6
Meter, Volt-ohm	Δ	л	Δ	Δ	X	л	1
Micro centrifuge				x	л		1
Microscope				X		х	2
Mixer, vortex				x		21	1
Oven				x			1
Oven, drying			x		х		2
Oven, laboratory	х	х	x	х	X	х	6
Pipettes		x			21		1
Pipettors		21	x	х		х	3
Polarimeter		х		x		x	3
Polymerase Chain Reaction apparatus				x			1
Pump, for water filtration					х		1
Pump, vacuum		х	х	х	x	х	5
Pycnometer						x	1
Refractometer			х			x	~
Refractometer, Abbe						x	1
Rotary evaporator		х		х			2
Shaker, temperature-controlled water bath					х		1
Soxhlet Extractor		х					1
Spectrometer, Fourier Transform Infrared		x	х		х	х	4
Spectrometer, Ultraviolet Visible		х	х	х	х	х	5
Spectrophotometer, Atomic Absorption			x	x			2
Spectrophotometer, Fourier Transform Infrared (with gas cell)						х	1
Spectrophotometer, I function infinite (what gas cell)					х		1
Spectrophotometer, Ultraviolet Visible			х	х			2
Spectrophotometer, Ultraviolet Visible scanning					х	х	2
Suction Flask		х					1
Tensiometer, Surface tension apparatus						х	1
,							<u> </u>

Commission on Higher Education Policies and Standards for BS Chemistry

Instrument	Gen Org Ana Bio Inorg	FREQ
Test tubes	X	1
Thermometer	Х	1
Thermometer, electronic	X X X	x 3
Ultraviolet lamp	Х	1
Viscometer	Х	x 1
Vortex mixer	Х	1
Water bath	Х	1

# Section 23 Safety

# 23.1 Staff

The Chemistry department should appoint qualified staff as a safety officer to take charge of the following:

- a. Chemical safety
- b. Maintenance of equipment and other chemistry facilities
- c. Chemical inventory
- d. First aid
- e. Emergency measures, including fire, earthquake, and others
- f. Security
- g. Chemical waste disposal

The safety officer shall be properly trained, instructed and equipped to oversee the various safety measures including waste disposal system. Schools shall ensure that safety officers undergo regular retraining and upgrading.

Laboratory safety officers shall be familiar with the emergency features of the laboratory and shall know the emergency procedures in cases of fires, accidents, earthquakes, and chemical spills. They shall be familiar with basic first aid procedures.

# 23.2 Safety and emergency fixtures and equipment

The Chemistry department must see to it that appropriate safety and emergency fixtures and equipment are available, easily accessed when needed and maintained regularly.

# 23.3 Staff training

The Chemistry department should hold special training and instruction for the staff and students and periodically hold drills involving staff and students.

## 23.4 Safety practices and measures

The Chemistry Department must implement at all times safety practices and measures in the laboratory.

Chemical waste must be disposed properly and in accordance with local environmental laws and regulations.

Safety measures are described in detail in Appendix B.

#### ARTICLE VIII ADMISSION AND RETENTION REQUIREMENTS

#### Section 24 Admission and Retention

The basic requirement for eligibility for admission of a student to any tertiary level degree program shall be graduation from the secondary level recognized by the Department of Education. Higher education institutions must specify admission, retention and residency requirements. They should ensure that all students are aware of these policies.

#### ARTICLE IX TRANSITORY, REPEALING AND EFFECTIVITY PROVISIONS

#### Section 25 Transitory Provision

HEIs that have been granted permit or recognition for Bachelor of Science in Chemistry program are required to fully comply with all the requirements in this CMO, within a non-extendable period of five (5) years after the date of its effectivity. State Universities and Colleges (SUCs) and Local Colleges and Universities (LCUs) shall also comply with the requirements herein set forth.

#### Section 26 Repealing Clause

All CHED issuances, rules and regulations or parts thereof, which are inconsistent with the provisions of this CMO are hereby repealed.

#### Section 27 Effectivity Clause

This CMO shall take effect fifteen (15) days after its publication in the Official Gazette, or in two (2) newspaper of national circulation. This CMO shall be implemented beginning Academic Year 2008-2009.

[HS3]For strict compliance.

Pasig City, Philippines, March 30, 2007

#### FOR THE COMMISSION

CARLITO S. PUNO, DPA Chairman

# APPENDIX A COURSE DESCRIPTIONS FOR SOME CHEMISTRY ELECTIVES

## **ORGANIC CHEMISTRY III, LECTURE**

#### **COURSE DESCRIPTION**

NUMBER OF UNITS: 3 units

PREREQUISITES: Organic Chemistry II Lecture and Laboratory

#### **COURSE OUTLINE**

The following are suggested topics that can be included in a third semester lecture course on Organic Chemistry:

- a. Advanced Spectroscopy
- b. Retrosynthesis
- c. Pericyclic Reactions
- d. Carbanion and Carbocation Chemistry
- e. Chemistry of Natural Products
- f. Heterocyclic Chemistry

# INDUSTRIAL CHEMISTRY

## **COURSE DESCRIPTION**

Learning Objectives

- a. The course aims to equip the student with the fundamentals of the chemical industry.
- b. To gain a firm understanding of the process of transfer of technology from the chemical laboratory bench to the actual commercial production of the chemical commodity.
- c. To gain a rudimentary, working knowledge of the following: unit operations, chemical process design, selection, and economics, research and development, product development, market evaluation, patents, environmental protection and waste management, and quality assurance systems.
- d. To give an overview of commodity products such as: agrochemical, food products, flavors and food additives, oils, fats and waxes, soaps and detergents, the sugar and polysaccharide industries, pulp and paper, polymer industry, petrochemicals, and the pharmaceutical industry.
- e. To discuss the impact of the chemistry profession on industry and society.

#### NUMBER OF UNITS: 3 units

**PREREQUISITES:** General Chemistry II Lecture and Laboratory; Organic Chemistry II Lecture and Laboratory; Analytical Chemistry I Lecture and Laboratory; Inorganic Chemistry Lecture

#### COURSE OUTLINE

Table A1. Topics for industrial chemistry and recommended number of hours.

Topic	Est. Hours*
I. The Chemist as a Professional in Industry	
1. The Industrial Organizational Set-up	1
2. Basic Chemical Data	2
3. Research and Development	2
4. Unit operations, Chemical Process Design, Selection, Economics,	3
and Operation	1
5. Product Development and Market Evaluation	2
6. Quality Assurance Systems, the ISO, Good Laboratory Practices	1
(GLP)	2
7. Patents and Chemical Jurisprudence	
8. Environmental Protection and Waste Management	
II. The Chemical Process Industries	
1. Agrochemical	2
2. Food products, flavors and food additives	2
3. Oils, fats and waxes, the coconut oil industry	2
4. Soaps and detergents	2
5. The sugar, starch, and seaweed polysaccharide industries	2
6. Pulp and paper	2
7. Wood Chemicals	2
8. Fermentation Industry	2
9. The Polymer Industry	2
10. Petrochemicals	2
11. Pharmaceutical industry	2
III. Case Studies and Plant Visits	
1. Selected case studies: commercialization of chemical commodities.	3
2. Plant visits.	Х
*Based on a 15 meab three credit hour course	

\*Based on a 15-week, three credit-hour course.

#### SUGGESTED TEXTS AND REFERENCES

Alloway, B. J. and Ayres, D. C. (1993) *Chemical Principles of Environmental Pollution*, Blackie Academic.

Basta, N. (1994) Shreve's Chemical Process Industries Handbook, 6<sup>th</sup> ed., McGraw-Hill.

- Clow, A. and Clow, N.L. (1992) The Chemical Revolution: A Contribution to Social Technology vol. 8, Gordon & Breach.
- Crone, H. D. (1986) Chemicals and Society: A Guide to the New Chemical Age, Cambridge University Press.

Drake (1992) Chemical Industry: Friend to the Environment? Vol. 103, CRC Press.

Emerson, W.S. (1991) Guide to the Chemical Industry: Technology, R & D, Marketing, & Employment, Krieger Pub. Co.

Heaton, A., (ed.) (1994) The Chemical Industry, 2<sup>nd</sup> ed., Routledge, Chapman & Hall.

American Society for Quality Control (1988) Quality Assurance for the Chemical & Process Industries: A Manual of Good Practices, ASQC Quality Press.

Prichard, E. (1995) Quality in the Analytical Chemistry Laboratory, John Wiley.

Rodman, D., Bly, D.D., Owens, F. and Anderson, A-C. (1995) *Career Transitions for Chemists*, American Chemistry Society.

Rueben, B. G. and Bursall, M. L. The Chemical Economy: A Guide to the Technology & Economics of the Chemical Industry, Books on Demand, undated. Shreve, R. N. and Brink Jr., J.A. (1977) *Chemical Process Industries, 4<sup>th</sup> ed*, McGraw-Hill.

## AGRICULTURAL CHEMISTRY

## **COURSE DESCRIPTION**

#### Learning Objectives

The course aims to provide a basic understanding and an appreciation of the role of chemistry in agriculture. The objectives of the course are:

- a. To enable the student to recognize the main groups of chemicals used in agriculture and relate their physiological and agronomic effects to their molecular structure and action.
- b. To understand the basic principles and applications of biotechnology to agriculture.

#### NUMBER OF UNITS: 3 units

**PREREQUISITES:** General Chemistry II Lecture and Laboratory; Organic Chemistry II Lecture and Laboratory; Analytical Chemistry I Lecture and Laboratory; Inorganic Chemistry Lecture

#### **COURSE OUTLINE**

- a. Chemicals used in Agriculture
- Fertilizers
- Pesticides in crop production
- Plant growth regulators
- b. Chemicals in Livestock Production
- Feed additives
- Pharmaceuticals
- c. Agricultural Biotechnology: Principles and Applications

## ADVANCED ANALYTICAL CHEMISTRY

#### **COURSE DESCRIPTION**

This course describes the practice of Analytical Chemistry as an information science, emphasizing statistics, introductory chemometrics and quality assurance.

#### **Number of Units:** 3

PREREQUISITES: Analytical Chemistry 2, Elementary Statistics

## **COURSE OBJECTIVES**

This course aims:

- a. To provide a deeper understanding of the principles and methods involved in the different phases of the analytical process, such as sampling, measurement, calibration and evaluation of the analytical data;
- b. To build mastery of the statistical methods which are used in the evaluation of the quality of analytical methods;
- c. To present the principles and methods of quality assurance in the analytical chemistry laboratory; and
- d. To introduce the principles and techniques of chemometrics, and their application in chemical measurements.

# **COURSE COMPETENCIES:**

By the end of the course, the student should be able to:

- a. Apply a number of statistical tests for the evaluation of the results of a chemical analysis;
- b. Formulate an appropriate sampling plan for an analytical problem;
- c. Determine and interpret the figures of merit for a method of chemical analysis;
- d. Employ quality control and quality assurance procedures;
- e. Make a valid experimental design for the development of a method of chemical analysis;
- f. Optimize the measurement parameters in a chemical analysis; and
- g. Apply pattern recognition and other nonparametric data analysis for obtaining information from the results of chemical measurements.

# **COURSE TOPICS**

# a. Introduction (3 hours)

Philosophy of analytical chemistry. Analytical problems. The analytical process. Quality Systems.

## b. Methods of chemical analysis (3 hours).

Absolute methods. Stoichiometric calculations. Philosophy of instrumentation. Instrumental methods.

## c. <u>Statistical evaluation of data (6 hours).</u>

Error analysis. Statistics of measurements. Significance testing – the Student t and F tests. Analysis of variance. Outliers.

# d. Principles of sampling (6 hours).

Importance of sampling. Sampling design: site, size, number. Statistical considerations. Sampling methods for gases, liquids and solids.

## e. Principles of measurement (6 hours).

Terminology. Figures of merit. Standardization of methods. Selection of analytical methods. Quality control methods. Control charts. Proficiency testing. Uncertainty.

# f. Principles of calibration (6 hours).

Basic concepts. Requirements for calibration. Modes of calibration. Frequency of

calibration. Modes of calibration. Linearity tests. Standard addition method. Calibration uncertainties. Traceability.

## g. Experimental design (6 hours).

Statistical design of experiments. Confidence and certainty. Design and selection of standards. Reference methods and validation. Method development.

## h. <u>Chemometrics (6 hours).</u>

Univariate and multivariate calibration. Optimization of experiments. Parameter estimation. Pattern recognition.

## SUGGESTED TEXTBOOKS

- Miller, J.C. and Miller, J.N. (2001) Statistics and Chemometrics for Analytical Chemistry, 4<sup>th</sup> ed., Prentice-Hall.
- Wedclawiak, B., Koc, W., and. Hadjicostas, E. (Eds). (2004) *Quality Assurance in Analytical Chemistry*, Springer-Verlag.
- Neidhart, B. and Weigscheider, W. (Eds). (2001) *Quality in Chemical Measurement*. Springer-Verlag.
- Kellner, R., Mermet, J.M., Otto, M., Valcarcel, M. and Widmer, H.M. (2004) *Analytical Chemistry: A Modern Approach to Analytical Science.* John Wiley & Sons.

Pritchard, E. (1995) Quality in the Analytical Chemistry Laboratory. John Wiley & Sons.

## SUGGESTED REFERENCES

Review papers from the following journals may be used: Analyst (UK), Analytical Chemistry (ACS), Analytica Chimica Acta (Netherlands), Journal of Chemical Education.

# INTRODUCTION TO THE CHEMISTRY OF NATURAL PRODUCTS

## **COURSE DESCRIPTION**

This course covers the different classes of natural products and their importance in health and commerce with emphasis on how chemical structures influence their physiological activities. It also includes the laboratory skills and techniques needed in the conduct of natural products chemistry research.

The course introduces the students to the applications and importance of natural products development for food, for perfumes and cosmetics, and for pharmaceutical and agricultural chemicals or extracts. Actual examples and case studies will be discussed.

This course aims to impart to chemistry students an understanding of their chemical structures and the way they are assembled by living organisms, as well as their biological properties, traditional uses and commercial potential.

## **NUMBER OF UNITS:** 3 units

## **COURSE OBJECTIVES**

The objectives of the course are:

- a. To understand the origin and classification of natural products;
- b. To appreciate the role of chemical structure in physiological function of natural products and their derivatives;

c. To introduce the applications and potentials of natural products as renewable and sustainable resources for food, medicines, and agriculture.

#### **COURSE COMPETENCIES**

At the end of the course, the students are expected to be able to:

- a. Recognize the different classes of natural products;
- b. Identify the major precursors of the different classes of natural products;
- c. Utilize appropriate techniques in the separation and identification of natural products; and
- d. Give and discuss applications and development of natural products as renewable and sustainable resources.

## PREREQUISITES: Organic Chemistry 2; Basic Biochemistry

## **COURSE TOPICS**

## a. Introduction to Natural Products Chemistry (3 hours)

- Sources
- o Terrestrial sources
- Marine sources
- Micro-organism sources
- o Animal Sources
- o Production by tissue culture and cell free systems
- o Other Sources
- b. Introduction to Secondary Metabolism (3 hours)

#### c. Metabolic pathways and major classes of natural products (30 hours)

- Acetate derivatives: fatty acids and polyketides (6 hours)
- Shikimate derivatives: flavonoids and polyphenols (6 hours)
- Isopentenyl pyrophosphate derivatives: terpenes and steroids (9 hours)
- Amino acid derivatives: Alkaloids (9 hours)

## d. Methods of Natural Products Analysis (6 hours)

- Separation techniques
- Characterization and identification techniques
- Bioassays

## e. Special topics (6 hours)

- The value of natural products
- Interactions mediated by natural products
- o Bioactivities of natural products
- Natural Products: Its Applications and Development as Renewable and Sustainable Resources
- o Medicine: pharmaceuticals, cosmeceuticals, microbial transformations
- o Food: nutraceuticals, nutrigenomics
- o Alternative applications: biocides
- Application of molecular biology and biotechnology to natural products.

#### SUGGESTED REFERENCES

#### Introduction, classes and value of natural products:

Mann, J. (1987) Secondary Metabolism. 2nd ed., Oxford Science Publication. Mann, J. (1994) Chemical Aspects of Biosynthesis, Oxford Science Publication. Dewick, P.M. (1997) Medicinal Natural Products: A Biosynthetic Approach.

## Methods of natural products analysis

Harborne, JB. (1984) Phytochemical Methods. A Guide to Modern Techniques of Plant Analysis. 2nd ed., Chapman and Hall.

Rahman, A., Choudhary, M.I., and Thomson, W.J. (2001) *Bioassay Techniques for Drug Development*, Harwood Academic Press, Amsterdam.

## Websites for Applications:

http://biotech.icmb.utexas.edu/botany/ - and links from this; contains interesting information on natural product compounds which are used in chemotherapy.

http://www.ars-grin.gov/duke/index.html - very useful, with searchable database

#### Journals

- a. Journal of Agriculture and Food Chemistry
- b. Journal of Natural Products
- c. Natural Products Reports
- d. Phytochemistry
- e. Phytochemical Analysis
- f. Phytochemistry Reviews
- g. Planta Medica
- h. Proceedings of the National Academy of Science, USA

## ENVIRONMENTAL CHEMISTRY

#### **COURSE DESCRIPTION**

The course introduces the student to the scientific principles and processes that govern the behavior of chemical species in the air, water, and soil environments and the influence of human activities on these processes.

Environmental chemistry aims to provide the student with a better understanding of the important chemical concepts that are involved in environmental processes, the critical role chemistry plays in environmental issues, and some of the ways that chemistry connects to other disciplines.

#### NUMBER OF UNITS: 3 units

#### **COURSE OBJECTIVES**

- a. Understand the basic principles of the behavior of both organic and inorganic compounds in the environment based on their chemical structure and reactivity;
- b. Understand fate and transport of chemicals in the environment, with emphasis on the atmosphere, hydrosphere, and soil environment;
- c. Have a good overview of the chemicals of concern;
- d. Gain a global perspective on environmental issues e.g. climate change, stratospheric ozone depletion, and environmental catastrophes.

# **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Apply basic chemical principles to environmental processes;
- b. Use critical thinking skills in evaluating environmental issues;
- c. Integrate social awareness and ethics in dealing with environmental issues.

# PREREQUISITES: Organic Chemistry 2, Analytical Chemistry 2

# **COURSE OUTLINE**

# a. Introduction (3 hours)

- Definition and overview of environmental chemistry; toxic organic substances; water chemistry; fuels and energy sources; green chemistry;
- The biogeochemical cycles (C, O, N, S, P and the hydrologic cycle)
- Unique properties of water

# b. The Chemistry of the Atmosphere (3 hours)

- The nature & composition of the atmosphere (regions of the atmosphere);
- Stratospheric chemistry and the ozone layer (photochemistry principles; ozone formation;
- Role of chemicals in ozone destruction (catalytic and noncatalytic ozone destruction, chlorofluorocarbons (CFCs), CFC replacements);
- Other stratospheric chemical processes; systematics of stratospheric chemistry

# c. Tropospheric Chemistry and Air Pollution (3 hours)

- Gas concentrations (interconversion);
- Chemistry of the troposphere (trace gases, principles of reactivity);
- Photochemical smog (origin, occurrence and reduction of smog);
- Acid rain; particulate matter; outdoor air pollution and health effects; indoor air pollution and health effects (formaldehyde, nitrogen dioxide, carbon monoxide, tobacco smoke, asbestos);
- Radioactivity from radon

# d. Greenhouse Effect & Climate Change (3 hours)

- Mechanism of greenhouse effect; greenhouse gases; global warming by other substances (trace gases, methane, nitrous oxide, CFCs and their replacements, ozone, aerosols); global warming predictions;
- The Montreal Protocol and Kyoto Protocol
- e. Toxic Organic Chemicals (7.5 hours)
- Pesticides; organochlorine insecticides (DDT accumulation and fate, DDT analogs, toxaphenes, cyclopentadienes); modern insecticides (organophosphates, carbamates, natural insecticides); herbicides (triazine herbicides, organic herbicides, phenoxy herbicides, dioxin contamination and sources);
- PCBs (structure, properties, uses); toxicology and health effects of PCBs, dioxins, and furans; toxic organic waste disposal;
- Polynuclear aromatic hydrocarbons (structure, PAHs as pollutants)

# f. The Chemistry of the Hydrosphere (7.5 hours)

- The properties and composition of natural waters: the CO2/carbonate system (acidbase equilibria; alkalinity indices; hardness index); dissolved oxygen; anaerobic decomposition; nitrogen compounds (nitrates, nitrites, nitrosamines);
- Water pollutants; water supplies and their contamination; purification of municipal water supplies; waste water treatment

# g. <u>The Chemistry of the Lithosphere (4.5 hours)</u>

- The chemistry of soil; soil microbial chemistry;
- Toxicity and bioaccumulation of heavy metals (mercury, lead, cadmium, arsenic); heavy metals in soils; sewage and sediments (soil chemistry, binding of heavy metals to soils, analysis and remediation of contaminated sediments)

# h. Hazardous Wastes: Reduction, Treatment and Disposal (4.5 hours)

• Management of toxic waste; waste reduction and minimization; recycling; physical methods of waste treatment; chemical treatment; photolytic reactions; thermal treatment; biodegradation; land treatment and composting; preparation of wastes for disposal; ultimate disposal of wastes; leachate and gas emissions; in-situ treatment

# i. Energy and the Environment (3 hours)

- Liquid and gaseous fuels (gasoline, natural gas, alcohol fuels);
- Hydrogen- fuel of the future (storage, production);
- Nuclear energy (fission and fusion reactors)

# j. Environmental Chemical Analysis (6 hours)

- The role and importance of environmental chemical analysis; classical methods; instrumental methods;
- Analysis of water samples; atmospheric monitoring; sampling vapors and gases; methods of analysis (sulfur dioxide, nitrogen oxides, oxidants, carbon monoxide, hydrocarbons, particulate matter); direct spectrophotometric analysis of gaseous air pollutants

## k. Green Chemistry (3 hours)

- The Twelve Principles of Green Chemistry;
- Application to industrial chemicals
- Case studies

## SUGGESTED TEXTBOOK

Baird, C. and Cann, M. (2004) *Environmental Chemistry*, 3<sup>rd</sup> ed., W.H. Freeman and Company, New York (2004)

## SUGGESTED REFERENCES

Spiro, T.G. and Stigliani, W.M. (2003) Chemistry of the Environment, 2nd ed., Prentice Hall.

Van Loon, G.W., and Duffy, S.J. (2000) *Environmental Chemistry, A Global Perspective*, Oxford University Press.

Manahan, S.H. (1994) Environmental Chemistry, 6th ed., Lewis Publishers.

- Anastas, P.T. and Warner, J.C. (1998) *Green Chemistry: Theory and Practice*, Oxford University Press, New York.
- Cann, M.C. and Connely, M.E. (2000) Real World Cases in Green Chemistry, American Chemical Society; Washington, DC.

#### **COMMENTS**

It is highly recommended that case studies be developed and used in the lecture, for discussions and debate, and/or for course-related research.

# MATERIALS SCIENCE

#### **OVERVIEW OF SUBJECT AREA**

Polymer and Materials Science are two interdisciplinary fields that are strongly founded in Chemistry. Polymer Chemistry specializes in the study macromolecules that are either synthetic or natural, and whose microstructure and properties are largely affected by the size of the molecule. A separate Polymer Chemistry (or Polymer Science) course is presently not required in the B. S. Chemistry curriculum but is already offered by many universities in the country as a 3-unit elective (Table 1). Materials Science (Materials Science and Engineering, Materials Science and Technology, or Materials Chemistry) is a broader field, which specializes in the study of metals, ceramics, plastics (polymers), semiconductors, and composites. This subject is also not required in the B. S. Chemistry program and is more commonly offered as a basic course for engineering students or as an elective for Chemistry students at the graduate level. These fields have increasingly become important in industry because of their broad application in the high-tech industry and in many common-day products such as plastics and electronic devices. Many developments in these fields also factor in nanotechnology.

The fact that these fields deal with something 'chemical' imply that the chemist is poised to make significant contribution in these fields, and this is in fact the case. However, there is a separate Materials and Engineering program, which is distinct from Chemistry or Physics because the former is largely themed on the concept of 'microstructure'.<sup>2</sup>

#### **OBJECTIVES OF SUBJECT AREA:**

These courses are not foundation courses for Chemistry and they need not be required in the basic curriculum for BS Chemistry. However, because of their increasing importance in emerging disciplines such as nanotechnology, and in research and development in industry,<sup>3</sup> it is highly recommended that the BS Chemistry graduate has significant exposure in these fields either through: (a) preferably, separate elective courses in Polymer Chemistry and Materials Science, or (b) incorporation of special topics in the foundation courses of Chemistry.

The general aims of the Materials Science subject area are for the student to:

- a. Acquire a clear understanding of the basic structure and properties of materials such as polymers, metals, ceramics, semiconductors, and their composites;
- b. Be able to distinguish the different levels of structure-property relationships as applied to understanding the properties and function of materials;
- c. Acquire an overview of the different processes in the production of materials and their present-day applications;

<sup>&</sup>lt;sup>2</sup> Cramb, A. W. *What it the Future Direction of Undergraduate Education in Materials Departments?* In <u>http://www.mrs.org/</u> (accessed May, 2006).

<sup>&</sup>lt;sup>3</sup> In the Philippines, major industries such as the paint and resins, packaging, electronics and semiconductors industry often hire B. S. Chemistry graduates in their technical laboratories.

- d. Gain experience in the measurement of materials properties such as viscosity, refractive index, and electrical conductivity;
- e. Gain an overview of synthesis methods applied to polymeric materials such as those used in the packaging industry, paints and coatings, and electronics packaging industry; and
- f. Acquire an overview of the advances in materials engineering and technology and nanotechnology.

#### RECOMMENDATIONS

One way of introducing materials science in the curriculum is by incorporating topics in appropriate core courses. Most modern textbooks in the foundation courses in Chemistry already incorporate a chapter related to Polymers or Materials, and these chapters may be used with additional supplementary topics from the more specialized textbooks.

For example, the following topics can be introduced in Organic Chemistry: macromolecular structure, molecular weights of polymers, examples of synthesis of polymers: radical polymerization/condensation polymerization, the basic chemical composition of different polymeric materials and their typical uses.

#### FUNDAMENTALS OF MATERIALS CHEMISTRY

#### **COURSE DESCRIPTION**

The course aims to provide the students a fundamental background on the structure and properties of materials. Topics include structure of amorphous and crystalline solids, X-ray diffraction, defects in solids, phase equilibria, kinetics of crystallization, diffusion in solids, mechanical properties of materials, electrical and optical properties, and materials processing & design.

NUMBER OF UNITS: 3 units

PREREQUISITES: Physical Chemistry 1, Inorganic Chemistry

#### **COURSE OBJECTIVES**

See "OBJECTIVES OF SUBJECT AREA" above.

#### **COURSE COMPETENCIES**

At the end of the semester, the student should be able to:

- a. Gain a clear understanding of the basic structure and properties of metals, ceramics, plastics (polymers), semiconductors, and composites;
- b. Be familiar with the crystalline state and their lattices; assign Miller indices; and understand defects structures: point, dislocations, and volume defects;
- c. Gain an overview of X-ray diffraction, microscopy, and other techniques for probing atomic and microstructure of solid materials;
- d. Learn the basics of mechanical properties in terms of stress-strain relationships, measurement techniques, and be able to differentiate classes of materials in terms of their mechanical properties;
- e. Learn the phase diagrams of materials and their use in processing such as alloying of metals and synthesis of ceramics;

- f. Gain an overview of polymeric structures and their viscoelastic properties; semiconductor structure, conducting polymers, electronic properties and device applications; electrical, optical, magnetic and thermal properties of materials and the measurement techniques;
- g. Gain an overview of composites, their design and properties, and sample applications; and
- h. Gain an overall understanding of the interplay between composition and microstructure, and general structure-property relationships as applied to the design and understanding of the functional properties of different materials.

# **COURSE TOPICS**

- a. Introduction / Overview of Materials Science & Engineering, Atomic Scale Structures (2 hours)
- b. Crystal Structures, Bravais Lattices, Miller Indices, X-ray diffraction, Point Defects and Diffusion (6 hours)
- c. Linear Defects and Plastic Deformation in Solids (3 hours)
- d. Amorphous solids: structure and properties (6 hours)
- e. Solid transformations in solids, phase diagrams (3 hours)
- f. Kinetics of crystallization (3 hours)
- g. Mechanical properties of solids: deformation, fracture, fatigue, creep, viscoelastic properties (3 hours)
- h. Survey of electrical, optical, and magnetic properties (9 hours)
- i. Thermal properties (3 hours)
- j. Composites (3 hours)
- k. Effects of environments on materials properties, corrosion, environmental impact (3 hours)
- 1. Materials synthesis and design (3 hours)
- m. Introduction to Nanotechnology

## REFERENCES

- Schaffer, J. P., Saxena, A., Antolovich, S. D., Sanders Jr., T. H. and Warner, S. B. (1995) *The Science and Design of Engineering Materials, Irwin, Intrenational Student ed*, (or latest edition)
- Callister Jr., W. D. (1997) *Materials Science and Engineering: An Introduction, 4<sup>th</sup> ed., John Wiley and Sons, Inc., (or latest edition)*

# COMMENTS

- a. A term paper or report is recommended to integrate all of the topics discussed in this course, as well as other chemistry courses.
- b. The course should use key and recent technical publications to ensure that it is up-todate with developments in the field.

# INTRODUCTION TO POLYMER CHEMISTRY, LECTURE AND LABORATORY (OPTIONAL)

## **COURSE DESCRIPTION**

This is an introductory course in polymer science and technology. Topics include: molecular weight and distribution, classes of polymers and their polymerization reactions and kinetics, amorphous and crystalline polymers, viscoelastic properties, mechanical and

thermal testing of polymers, polymer processing technologies, specialty and engineering polymers, stability and degradation and environmental impact of plastics.

#### NUMBER OF UNITS: LECTURE: 3 UNITS; LABORATORY (OPTIONAL): 1 OR 2 UNITS

#### **COURSE OBJECTIVES**

See Subject Area for Materials Chemistry.

#### **COURSE COMPETENCIES**

At the end of the semester, the student should be able to:

- a. Gain a clear understanding of the basic structure of macromolecules, their molecular weight distributions and be able to calculate average molecular weights;
- b. Be familiar with the amorphous and crystalline states polymers;
- c. Learn the different methodologies for characterizing the molecular weights of polymers such as light scattering techniques, colligative properties, and gel permeation chromatography;
- d. Learn the basics of mechanical properties particularly the viscoelastic nature of polymers materials, their modeling, and be able to relate the viscous and elastic response to the structure of the polymers;
- e. Gain an overview of the classes of polymers and their polymerization techniques, the kinetics of various polymerization techniques such as radical polymerization, stepgrowth polymerization, ionic polymerization, and copolymerization;
- f. Gain an overview of the methods to characterize polymers: molecular weight, mechanical, thermal, optical, and electrical properties;
- g. Gain an overview of polymer processing methodologies such as molding and extrusion; learn the functional properties of engineering polymers, their degradation, stability, and environmental impact, recycling, and other related issues; and
- h. Gain an overall understanding of the interplay between composition and microstructure, and general structure-property relationships as applied to the design and understanding of the functional properties of polymeric materials.

**PREREQUISITES:** Physical Chemistry 1 (may be a co-requisite), Organic Chemistry 2

## **COURSE TOPICS (NUMBER OF HOURS):**

- a. Introduction and overview (2 hours)
- b. Structure of polymers: classes, stereochemistry, morphology (5 hours)
- c. Polymer Molecular Weight: Calculation and Measurement (4 hours)
- d. Radical Polymers: classes, polymerization techniques, and kinetics (4 hours)
- e. Step-growth polymers: classes, polymerization, kinetics (4 hours)
- f. Ionic polymerization: living polymers, cationic and anionic polymerization (3 hours)
- g. Viscoelastic Properties of Polymers: mechanical and physical testing, structureproperty relationships (9 hours)
- h. Thermal properties and characterization (5 hours)
- i. Survey of Specialty and Engineering Polymers (4 hours)
- j. Overview of Polymer Processing Technologies (3 hours)
- k. Polymer Degradation and Stability, Environmental Impact (3 hours)

#### LIST OF SOME SUGGESTED EXPERIMENTS:

- a. PMMA synthesis by solution radical polymerization
- b. PMMA synthesis by cationic polymerization

- c. Crosslinked PMMA synthesis
- d. Polystyrene synthesis by cationic polymerization
- e. Measurement of viscosity molecular weight
- f. Measurement of polydispersity index by gel permeation chromatography
- g. Infrared spectroscopy of polymers
- h. NMR characterization of polymer
- i. Emulsion polymerization
- j. Measurement of glass transition temperature by differential scanning calorimetry
- k. Thermogravimetric analysis
- 1. Dynamic mechanical properties of polycarbonate
- m. Modification of Biopolymers (Cellulose and effect of crosslinking)
- n. Condensation Polymerization (phenol-formaldehyde)
- o. Synthesis of Polyaniline, a Conducting Polymer
- p. Mechanical Properties: Creep and Stress-relaxation

#### SUGGESTED REFERENCES

Latest editions of:

- a. Askadskii, A. A. Physical Properties of Polymers: Prediction and Control, 1/e. Gordon and Breach, 1996.
- b. Brent Strong, A. Plastics: Materials Processing, 2/e. Prentice Hall, 1999.
- c. Cowie, J. M. G. Polymers: Chemistry and Physics of Modern Materials, 2/e. Chapman and Hall, 1991.
- d. Miller, R., M. Miller, and E. A. Tury (eds.). Thermal Characterization of Polymeric Materials. Academic Press, 1997.
- e. Odian, G. Principles of Polymerization, 3/e. John Wiley, 1991.
- f. Rosen, S. L., Fundamentals of Polymeric Materials, 2/e. John Wiley & Sons, 1993.
- g. Sandler, S., W. Karo, J. Bonesteel, E. Pearce, Polymer Synthesis Characterization: A Laboratory Manual, Academic Press, 1998.
- h. Young, R. J. and P. A. Lovell. Introduction to Polymers. Chapman and Hall, 1991

## INTRODUCTION TO COMPUTATIONAL CHEMISTRY

#### INTRODUCTION

During the past 50 years, many theoretical techniques in quantum and statistical mechanics have been developed and made into standard computational procedures. These help elucidate the explanation of chemical phenomena. Oftentimes, these techniques have provided extra support for hypotheses that are a result of experimental data. But there have also been instances where the results of such theoretical techniques predicted phenomena prior to experimental confirmation. In all cases, these theoretical and computational techniques have reached a level of predictive accuracy. In a few years, knowledge of these techniques will not only be considered an extra tool, but a necessary one within the scientific method of explaining natural phenomena.

Computational chemistry uses the results of theoretical chemistry, such as the Schrodinger Equation, and incorporates them into computer programs to calculate the structures and properties of molecules in order to solve real chemical problems. Examples of such properties are minimum energy structures, structure and energy correlations, charges, dipoles, vibrational frequencies, and spectroscopic quantities. Computational chemistry includes electronic structure calculations and simulation methods using Monte Carlo or Molecular Dynamics Techniques.

# **COURSE DESCRIPTION**

This course focuses on the basic principles of computational chemistry. Both molecular mechanical and quantum mechanical models are covered. A general survey of the important techniques will be presented, followed by theoretical and practical aspects of some of the more important techniques. This course is a stand-alone three-unit course with 2 units of lecture and 1 unit of lab.

#### NUMBER OF UNITS:

This may be delivered as a 3-unit lecture course, or be divided into a 2-unit lecture course and 1-unit computer laboratory course.

#### **COURSE OBJECTIVES**

This course aims to provide the student with enough knowledge of the basic techniques in computational chemistry in order for them to use these techniques as an additional tool to their research work.

## **COURSE COMPETENCIES**

At the end of the course, the student should be able to:

- a. Understand different computational techniques;
- b. Apply the appropriate technique appropriate to a problem; and
- c. Install, set-up and run computational programs using the Linux operating system.

## **PREREQUISITES:** Physical Chemistry 3

#### **COURSE TOPICS (NUMBER OF HOURS):**

Depending on the availability of time, Optional topics may be covered. There are enough topics in this outline to fill two semesters with a lecture-laboratory combination.

## a. Introduction to Computational Chemistry (3 hours)

- Newton's equations of motion.
- Fundamental equations of forces and potentials.
- From *ab initio* to molecular mechanics. The importance of assumptions.
- An overview of computational techniques and algorithms.

## b. Ab Initio calculations (3 hours)

- Review of Quantum Mechanics
- The Born-Oppenheimer Assumption
- The Slater Determinant
- The Hartree-Fock Equations and the Self-Consistent Field Approach
- Basis Sets
- Electron Correlation

## c. Optional topics:

- Configuration interaction
- Many-body perturbation theory
- Coupled-cluster methods
- Valence Bond Theory
- Extrapolation methods (G2, G3, CBS)
• Basis set superposition error

# d. Density Functional Theory (1.5 hours)

- Introduction to Functional Theory
- The Density Matrix
- The Kohn-Sham Equations
- The Basic Functionals Used in DFT

# e. Installing Linux, GAMESS, and GHEMICAL-GMS (3 hours)

## f. Lecture and Laboratory Exercises using HF and DFT (6 hours)

- Single-point energy calculation
- Geometry optimization
- Potential energy surface determination
- Normal mode analysis
- Electrostatics
- Thermodynamic properties
- Transition State Theory
- Comparison of the different techniques

# g. <u>A Survey of Semi-Empirical Methods: (3 hours)</u>

- Assumptions
- Advantages and disadvantages of each technique
- Multi-level techniques

# **Optional topics:**

- Solvation models
- Differential overlap treatment (From ZDO to MNDO)
- Improvements to DO (AM1, PM3 and SAM1)
- Hückel and Extended-Hückel Theory
- Quantum mechanics of the solid state

## h. Molecular Mechanics and Force Fields (3 hours)

- Interatomic and intramolecular potential energy functions
- Survey of the more popular force fields
- Energy minimization methods

## i. <u>Molecular Dynamics (6 hours)</u>

- Newton's equations of motion
- Integration
- Boundary conditions
- Cut-offs and neighborhood lists
- Electrostatics: The Ewald summation
- Constraint dynamics
- Equilibration
- Simulated annealing
- Statistical thermodynamics
- Radial distribution functions
- Introduction to correlation functions

# j. Monte Carlo (1.5 hours)

- The Monte Carlo algorithm
- Comparison with molecular dynamics

# k. GROMACS or NAMD (1.5 hours)

- Installation
- Input File System

### 1. Laboratory exercises using molecular dynamics (6 hours)

- Setting up a molecular dynamics calculation
- PDB file system

## m. Docking (1.5 hours)

### n. AutoDock and AutoDockTools (1.5 hours)

- Installation
- Input file system

### o. Laboratory exercises using AutoDock (3 hours)

- Optional topics:
- Drug design and chemoinformatics
- Quantitative structure-activity relationships
- Combinatorial libraries

### REFERENCES

Leach, A.R. (2001) *Molecular Modelling: Principles and Applications, 2<sup>nd</sup> ed.*, Prentice Hall. Jensen, F. (1998) *Introduction to Computational Chemistry*, John Wiley and Sons Inc.

Cramer, C.J. (2004) Essentials of Computational Chemistry: Theories and Models, 2<sup>nd</sup> ed., John Wiley and Sons Inc.

## **COMMENTS**

### Computer laboratory requirements

- a. This course requires a computer lab, ideally with one computer per student. Some of the sessions will be held in the classroom, while others will be held in the computer laboratory.
- b. It would also be ideal for a computer cluster where students can submit their computation jobs. One good startup cluster can be purchased from Tyan (Typhoon PSC (B2881) Dual AMD Opteron System, http://www.tyan.com/products/html/typhoon\_b2881.html).

### RECOMMENDATIONS

- a. A good background in biochemistry is desirable but not necessary
- b. The student should have a basic knowledge on how to use a computer. No prior knowledge of LINUX is required.
- c. The student's performance should be based on examinations and a computational project, which may be done individually or as a group with no more than four students per group. The topics are to be agreed upon by the professor and the student (group). Preferably, the topic should be closely related to the current thesis topic of the student (for the seniors). The projects will be submitted by the end of the semester.

### APPENDIX B CHEMICAL SAFETY

### **INTRODUCTION**

Safety is a prime concern in the chemical laboratory. In addition, special attention and consideration should be given because students are often not aware of the precautions that must be observed in the chemical laboratory. These Guidelines are divided into the following parts:

- a. BASIC SAFETY REQUIREMENTS This section covers guidelines on design of the laboratory and other safety features.
- b. SAFE LABORATORY PRACTICE This section covers recommendations on proper laboratory techniques and procedures.
- c. EMERGENCY PROCEDURES
- d. CHEMICAL STORAGE AND DISPOSAL

For further information, please consult handbooks on chemical safety. The following references were used for this set of recommendations: 1. Laboratory Chemical Hygiene Program-Health and Safety Training Program. Fermical, Inc., U.S.A.; 2. Safety with Merck. Merck Co., New Jersey.

### **Basic Safety Requirements**

- a. General Laboratory Design
  - 1. Adequate lighting is essential for a safe laboratory and efficient performance.
  - 2. Allow proper storage space for flammable and waste materials.
  - 3. Provide sufficient shelving or cabinets. No chemicals, apparatus or equipment should be stored or placed on the floor.
  - 4. All benches and tabletops must be impervious to chemical spills.
  - 5. Compressed gas cylinders should be strapped or chained to the wall or stable table and placed out of the main traffic flow.
  - 6. There should be sufficient workspace available for each student.
  - 7. The laboratory must be adequately ventilated. A large numbers of common substances present acute respiratory hazards, and should not be used in large amounts in a confined area. They should be dispensed and handled only when there is adequate ventilation.
  - 8. There should be a sufficient number of chemical fume hoods.
  - 9. Do not place extension cords on the floor or across aisles.
  - 10. Emergency deluge showers and eyewash fountains should be placed at easily accessible locations. Clear access to showers and eyewashes should be maintained at all times.
  - 11. Fire extinguishers should be strategically placed and clearly marked.
  - 12. Fire exits should be strategically located and be clearly marked. Building maps showing location of fire exits should be clearly posted in various places. (It must be possible to open fire exits from inside the building without a key.)
  - 13. Gas cylinders should be stored in appropriately ventilated cabinets or in open storage areas.
- b. Laboratory Supervision
  - 1. Laboratory safety is the responsibility of the institution. Each chemistry

department / institute should appoint a safety officer whose responsibility it is to oversee the various safety measures.

- 2. All laboratory activity should be properly and adequately supervised. Laboratory teaching courses should have an adequate supervisor: student ratio. Students doing advanced laboratory courses (for example, thesis projects) should not be allowed to work alone.
- 3. Laboratory supervisors should be familiar with the emergency features of the laboratory and should know the emergency procedures in cases of events such as fire, earthquake, and chemical spills. They should be familiar with basic first aid procedures.
- 4. Laboratory supervisors should be familiar with the experimental procedures and chemicals being used.
- 5. Wherever possible, avoid or minimize the use of concentrated reagents, volatile solvents, toxic and other dangerous chemicals. Whenever such chemicals are to be used, extra precaution should be observed.

### Safe Laboratory Practice

- a. Management of Work Space and General Equipment Set-up
  - 1. Keep workspace uncluttered.
  - 2. Set up clean, dry apparatus, firmly clamped and well back from the edge of the lab bench. Have due regard to the proximity of reagent bottles to burners, other workers, and their equipment. Choose sizes that can properly accommodate the procedure or operations to be performed, allowing at least 20% free space.
  - 3. Be sure that your glassware and equipment are free from flaws such as cracks, chips, and obvious defects. Chipped or cracked glassware should be repaired or discarded.
  - 4. Glass stopcocks in burets and separatory funnels should be freshly lubricated prior to use. Separatory funnels should be properly supported and oriented so that the stopcock will not be loosened by gravity. A retainer ring should be used on the stopcock plug.
  - 5. Condensers should be properly supported with securely positioned clamps. The attached water hoses should be secured with wire or a clamping device.
  - 6. Apparatus attached to a ring stand should be placed such that the center of gravity of the system is centered over the base with adequate provision for removing burners or baths quickly. Stands bearing heavy loads should be firmly attached to a bench top. Equipment racks should be securely anchored at the top and bottom.
  - 7. A pan properly placed under a reaction vessel or container can confine spilled liquids in the event of glass breakage.
  - 8. Fume hoods are recommended for all hazardous operations or whenever hazardous gases, vapors, mists or fumes are likely to be evolved. They are particularly necessary when working with flammable vapors with a density greater than air. Heavy vapors can settle on the bench top or floor, where they may use diffuse to a distant burner or ignition source.
  - 9. Hoods should be operating properly and must be free from any obstacles that prevent proper air movement.
  - 10. Use a hood when conducting a reaction that can result in an explosion or when using a vacuum system, which may implode. Close the hood sash to provide a shield. If a hood sash is not available, use a standing shield stabilized with weights or fasteners. Proper eye and face protection, including goggles and a face

shield must also be worn even when using a standing shield to a hood with a closed sash.

- 11. Chemicals should only be heated in a ventilated area or hood. Prior to heating a liquid, place boiling stones in reaction vessels that cannot be stirred. If a burner is to be used, distribute the heat with ceramic wire gauze. Use a thermometer in a boiling liquid if there is a risk of an exothermic decomposition. The set-up should allow for quick removal of heat.
- 12. When working with flammable gases or liquids, do not allow burners, switches, unshielded motors or other ignition sources in the vicinity. Use appropriate traps, condensers or scrubbers to minimize release of material in the environment. If a hot plate is used, ensure that its temperature is maintained below the auto-ignition temperature of the chemicals being handled or likely to be released.
- 13. Whenever possible, use electrical heaters instead of gas burners.
- b. Personal Safety
  - 1. Wear proper eye protection. Contact lenses should not be worn.
  - 2. Always know the hazards and physico-chemical properties of the chemicals used, e.g., corrosiveness, flammability, reactivity, and/or toxicity. Follow hazard precautions.
  - 3. Wear appropriate protective clothing and footwear. Full lab gowns made of cotton are preferred to aprons. Do not wear high-heeled shoes, sandals or slippers. Lab gowns should be removed when outside the laboratory.
  - 4. Confine long hair and loose clothing. Jewelries and similar accessories should be removed when working in the laboratory.
  - 5. Never work alone in the laboratory. Make sure somebody is around especially when handling hazardous substances.
  - 6. Do not eat, drink, smoke, use medication, or apply cosmetics in the chemical laboratory or storage areas.
  - 7. Do not perform unauthorized work, preparations, and experiments. Follow prescribed directions. If in doubt, ask you instructor.
  - 8. Always wash hands, arms and face before leaving the work area. This should be done even if gloves are used.
  - 9. Never engage in pranks or other acts of mischief.
  - 10. You should know the location of the fire extinguisher, fire escape, safety shower and first aid kit.
  - 11. Clean up all spills, broken glassware, etc., immediately.
- c. General Precautions for Handling Chemicals

All chemicals are potentially harmful. Avoid direct contact with any chemical. Some substances now considered to be non-hazardous may, in the future, be found to cause illness. It is especially important to keep chemicals away from hands, face, and clothing, including shoes. Many substances are readily absorbed through intact skin and inhalation. Chemicals can also enter the body, through the mouth, and by contamination of the hands. Chemicals can also be transferred to the eyes from the hands.

- 1. Do not use or handle any chemical until you have read and understood the label and Material Safety Data Sheet (MSDS) for that chemical.
- 2. All containers of chemicals must be clearly labeled. Do not use any substance from an unlabeled or doubtfully labeled container.
- 3. Keep your hands and face clean. Wash thoroughly with soap and warm water

whenever a chemical contacts your skin. Always wash you hands and arms before leaving the work area.

- 4. Never taste a chemical. If it is necessary to smell the chemical, cautiously waft a handful of vapor toward the nose. Smoking, drinking, eating, taking medication, and applying cosmetics is forbidden in chemical work or storage areas.
- 5. Some solvents, such as dimethyl sulfoxide (DMSO), serve as vehicles for the rapid transport of other substances into the skin. Always wear impervious gloves when handling such materials.
- 6. Many by-products of chemical reactions can be very hazardous. Planning for the handling and control of these toxic by-products should be part of the experimental procedure.
- d. Safe Laboratory Techniques
  - 1. Work neatly.
  - 2. Study the experimental procedures beforehand. Familiarize yourself with the chemicals, materials and apparatus to be used.
  - 3. Always add a reagent slowly. Swirl and observe what happens when the first small amount is added. Wait a few moments before adding more; some reactions take time to start.
  - 4. When adding liquids or powders, point the opening of a container away from yourself and away from others. Use a funnel when pouring liquids or powders into a small neck opening. Use a stirring rod to direct the flow of the liquid being poured.
  - 5. In case a stopper or lid is stuck, using extreme caution when opening the container. Wear gloves and tap the neck of the container lightly to loosen the stopper or lid.
  - 6. Never look down the opening of a vessel.
  - 7. To avoid violent reactions and spattering while diluting chemicals, always pour concentrated solutions slowly, while stirring, into water or into less concentrated solutions to allow any heat evolved to dissipate. Do not add water to concentrated acids as this may cause splattering; instead, add the acid to the water. Wear a face shield or splash goggles.
  - 8. When using a separatory funnel with a ground glass stopcock, ensure that the stopcock has been freshly lubricated and is closed. Keep a breaker under the funnel in case the stopcock fails.
  - 9. Large flasks must always be supported both at the neck and at the base during use, such as when heating with a Bunsen burner.
  - 10. Never use mouth suction to fill a pipette. Use an aspirator bulb or a loose-fitting hose attached to an aspirator. Constantly watch the tip of the pipette and do not allow it to draw air. Do not allow solutions to contaminate the aspirator bulb.
  - 11. When carrying large bottles of corrosive, toxic, or flammable liquids, use impact resistant transport containers to protect them from breakage and to contain spillage. Carry large bottles (e.g. 1 gallon) with both hands; do not hold than by the neck alone.
  - 12. Do not use diethyl ether in the presence of an open flame. Diethyl ether boils at around 36°C, which is comparable to our normal room temperature.
  - 13. In general, electric heaters are preferred to gas burners.
  - 14. Keep drawers and cabinets closed while working.
  - 15. Do store materials, especially chemicals, on the floor -- even temporarily.
  - 16. Work spaces and storage areas should be kept clear of broken glassware, leftover

chemicals, paper, dirt and debris.

- 17. Keep aisles free of obstructions such as pallets, carts, cylinders and bottles of chemicals, boxes and waste receptacles.
- 18. Avoid slipping hazards by keeping the floor clear of ice, stoppers, glass beads, glass rods and spilled liquids.
- 19. Use the required procedure for the proper disposal of chemical wastes, biological wastes and solvents.
- e. Use of Glassware
  - 1. Borosilicate glassware is recommended for all laboratory glassware, except for special experiments that use UV or other light sources. Generally, soft glass is used only in some reagent bottles, measuring glassware, stirring rods and glass tubing. Any sizable non-spherical glass equipment to be evacuated, such as suction flasks, should be heavy walled.
  - 2. Dewar flasks and large vacuum vessels should be taped, otherwise screened or contained in metal jackets to prevent flying glass resulting from an implosion. Thermos bottles, with thin walls are not to be substituted for Dewar flasks.
  - 3. All glass tubing and rods should be fire polished before use. Unpolished cut glass is sharp and can lacerate the skin, and can cut into stoppers and rubber hoses. Allow ample time for cooling to prevent burning the skin.
  - 4. When available, ground glassware is preferable. Glass stoppers and joints should be clean, dry and lightly lubricated. Rubber or cork stoppers should fit so that 1/3 to 1/2 of the stopper is inserted into the joint.
  - 5. When drilling a stopper, use a sharp borer, one size smaller than that which will just slip over the tube to be inserted. For rubber stoppers, lubricate with water or glycerol. Preferably, drill only part way through, and then finish by drilling from the opposite side. Discard a stopper if a hole is irregular, is cracked, does not fit the inserted tube snugly, or if it leaks.
  - 6. Protect your hands with cloth or leather gloves when inserting glass tubing and rods.
  - 7. Preparation of glass tubing: To cut glass tuning, hold the tubing against a firm support and make one quick firm stroke with a sharp triangular file or glass cutter. Cover the tubing with cloth and hold the tubing with both hands, with the nick centered between the hands. Place your thumbs on the tubing opposite the nick and push out the tubing. If the tubing does not readily pull apart, make a fresh sharp file scratch in the same place and repeat the operation. Be careful in cutting a short piece from a long piece of tubing because the long end may whip and injure a nearby person.
  - 8. Cleaning glassware: Clean glassware at the laboratory sink or in laboratory dishwashers. Use hot water (if available) and soap or other detergents if necessary. Use brushes of suitable stiffness and size. Avoid accumulating too much glassware in the clean-up area. The workspace around the sink is usually limited and piling of glassware lead to breakage. To minimize breakage of glassware, sinks should have rubber or plastic mats on their bottoms but not over the drains.

Avoid using strong chemical cleaning agents such as nitric acid, chronic acid, sulfuric acid, strong oxidizers or any chemical with "*per*" as a prefix in its name such as perchloric acid and ammonium persulfate, unless specifically instructed to do so, and only when wearing proper protective equipment.

- f. Use of Compressed Gases
  - 1. Handle cylinders of compressed gases as high-energy sources and therefore as potential explosives.
  - 2. Individually restrain cylinders of all sizes, empty or full, by straps, chains or cradles to prevent falling.
  - 3. Store cylinders in appropriately ventilated cabinets or in open storage areas.
  - 4. When storing or moving cylinders, have the protective caps securely in place to protect the valve stems. When moving large cylinders, strap them to properly designed wheeled carts to ensure stability.
  - 5. Do not expose cylinders to temperatures higher than 500°C. Some rupture devices on cylinders will release at about 650°C. Some small cylinders such as lecture bottles are not fitted with rupture devices, and many explode if exposed to high temperatures.
  - 6. Never use cylinders that cannot be identified positively.
  - 7. Never lubricate, modify, force or tamper with cylinder valves.
  - 8. Use toxic, flammable or reactive gases only in fume hoods.
  - 9. Never direct high-pressure gases at a person.
  - 10. Do not use compressed gas or compressed air to blow away dust or dirt.
  - 11. Be aware that rapid release of a compressed gas will cause an unsecured gas hose to whip dangerously. It may also build up a static charge that can ignite a combustible gas.
  - 12. Do not extinguish a flame involving a highly combustible gas until the source of the gas has been shut off; otherwise it can re-ignite and cause an explosion.
  - 13. Close the main cylinder valves tightly when not in use.
  - 14. Use the appropriate regulator on each gas cylinder. Adapters or homemade modifications are not advisable.
  - 15. Do not put oil or grease on the high-pressure side of an oxygen, chlorine or other cylinder of oxidizing agent. An explosion can result.
  - 16. Wear safety glasses when handling or using compressed gases.
  - 17. Do not bleed cylinders completely empty. Leave a slight pressure to keep contaminants out.
  - 18. Observe the following special rules when working with acetylene cylinders:
    - i. Acetylene cylinders are partially filled with acetone; always store upright.
    - ii. Do not use an acetylene cylinder that has been stored or handled in a nonup right position. Keep it in an upright position for at least 30 minutes prior to use.
    - iii. Ensure that the outlet line of an acetylene cylinder is protected with a flash arrestor.
    - iv. Never exceed the pressure limit indicated by the warning red line of acetylene pressure gauze.
    - v. Use only the correct type of tubing with gaseous acetylene. Tubing materials such as copper and some brass alloys form explosive acetylides.

### **Emergency Procedures**

- a. General Procedures for Spills
  - 1. Immediately alert fellow workers and supervisor.
  - 2. Avoid skin contact and minimize inhalation. All contaminated clothing must be removed immediately to prevent skin penetration. The skin must be washed with

soap and water. Continue flushing the skin with water for 15 minutes or more. Clothes should be laundered separately from the other clothing before reuse.

- 3. If the material is not particularly volatile, has a low order of toxicity, and there is no fire hazard, proceed clean-up operations as directed in the MSDS. To facilitate cleaning up of liquids, and if applicable, use an absorbent material that will neutralize the liquids (trisodium phosphate, sand followed by sodium bicarbonate solution (powder for acids), sodium thiosulfate for bromine, etc.).
- 4. A dustpan and brush should be used, and protective gloves should be worn. Clean the contaminated area with soap and water, and mop it dry. If the spill is on the floor, some absorbent should be sprinkled on the spot to prevent slipping. Dispose of the residue properly.
- 5. If a volatile, flammable or toxic material is spilled, warn everyone immediately to extinguish flames and turn off spark-producing equipment. Shut down all equipment and vacate area until it is decontaminated.
- 6. Many small liquid spills (<100 mL) can be absorbed with paper towels, sand or an absorbent. However, paper towels are not suitable for cleaning up flammable spills. Most solid spill can be brushed up and disposed of in appropriate solid waste containers, but care must be exercised to avoid reactive combinations. Do not leave paper towels or other materials used to clean up a spill in open trashcans in the work area. Dispose them properly.
- 7. Spills of Specific Type of Chemicals
- 8. Acids and other Acid Materials
- 9. Use calcined absorbent products. Avoid contact with skin. Do not clean-up hydrogen flouride (hydrofluoric acid, HF) with silica-containing materials such as sand or vermiculite.
- 10. Mercury
- 11. Because of the high toxicity of mercury vapor, spilled mercury should be cleanedup immediately and thoroughly using an aspirator or a vacuum device. Domestic vacuum cleaners must not be used because they will only re-disperse mercury aerosols and spread contamination. Mercury spilled into floor cracks can be made non-volatile by amalgamation with zinc dust.
- 12. Alkali Metals
- 13. A spill of alkali metal should be smothered with powdered graphite and removed to a safe location where it can be disposed of by reaction with a long chain primary alcohol such as n-butyl alcohol. Sodium-potassium alloys present even greater hazards than either sodium or potassium alone. Strict observation of supplier's recommendations must be followed. Particles of alkali metal splattered on the skin should be removed immediately. Flush the skin quickly with cool water. If any metal on the skin becomes ignited, deluge it with cold water immediately.
- 14. White (Yellow) Phosphorous
- 15. A spill of white phosphorous should be blanketed with sand or wet absorbent. If any white phosphorous is splattered on the skin, flush the skin with cool water and remove adhering phosphorous.
- b. Chemicals on the Skin
  - 1. For spills covering a small amount of skin, flush immediately with water for 15 minutes or more. Remove any clothing or jewelry adjacent to the spilled area to facilitate removal of any residual materials. Check the MSDS to determine whether any delayed effects should be expected. If a delayed reaction is noted,

seek medical attention immediately.

- 2. For larger spills, quickly remove all contaminated clothing, shoes, jewelry, etc. while using the safety shower. Do not attempt to wash off chemicals from contaminated clothing. Instead, remove the clothing quickly; no time should be wasted because of modesty. Be careful not to spread the chemical on the skin, or especially into the eyes. Unless the eyes are affected, do not remove safety goggles until all chemicals are washed from the hair and face. Use caution when removing shirts to prevent contamination of the eyes. It may be better to cut the garments off. Immediately flood the affected body area with cool water for at least 15 minutes. Resume if pain returns. Do not use creams or lotions. Get medical attention as soon as possible.
- c. Chemicals in the Eyes

For chemical splashes, the following are recommended: flushing of the eye for a minimum of 20 minutes, flushing the eye with copious amount of water, and checking for and removing contact lenses at once. Eyeballs should be rotated so that all surfaces are rinsed. Forcibly hold the eyelids open, if necessary. Call for emergency medical assistance at the first opportunity.

d. Releases of Acutely Toxic Vapors and Gases

Some vapors and gases can be permanently disabling or lethal when inhaled even at low concentrations. These include the following:

Fluorine, F2	Hydrogen cyanide, HCN
Chlorine, Cl2	Other Cyanides
Bromine, Br2	Methyl isocyanate, CH3NCO
Iodine, I <sub>2</sub>	Phosgene, COCl2
Arsine, AsH3	Phosphorous trichloride, PCl3
Stilbine, SbH3	Phosphorous oxychloride, POCl3
Hydrogen fluoride, HF	Phosphorous tribromide, PBr3
Hydrogen Sulfide, H <sub>2</sub> S	

If you plan to work with any of these chemicals, consult the MSDS and obtain additional guidance on emergency, first aid and handling procedures before you begin working with the chemical.

### **Chemical Storage and Disposal**

- a. Storage of Chemicals
  - 1. Storage of large reagent containers should be kept to a minimum. They should be stored on a low shelf, preferably in a tray adequate to contain spills and leakage. Do not store liquids above waist level. Incompatibles should not be stored in close proximity with each other.
  - 2. Chemicals that react with water should be stored away from water sources, aqueous chemicals and fire sprinklers.
  - 3. Corrosive materials should not be stored above waist level.
  - 4. Non-flammable safety cans are to be provided for quantities of flammable solvent larger than one gallon. If chemical purity requirements preclude the use of metal containers, the alternative is to place the glass container inside a metal container, and store in an approved flammable liquid storage cabinet or room.

- 5. Refrigerators. Storage of oxidizers and flammable chemicals in refrigerators constitutes a unique hazard since various control switches and defroster heaters can spark and ignite flammable materials resulting in an explosion or fire. Domestic refrigerators should never be used for storage of volatile chemicals.
  - i. Chemicals stored in refrigerators should be sealed, double packaged if possible, labeled with the name of the material and the date placed in the refrigerator, and the name of the person who stored the material. A current inventory should be maintained. Old chemicals should be disposed or after a specified storage period.
  - ii. Food should never be stored in a refrigerator used for chemical storage. These refrigerators should be clearly labeled "No Food."

### b. Disposal of Chemicals

Government and local environmental regulations should govern the disposal of laboratory wastes. In the absence of such guidelines, the following procedures should be observed:

- 1. To minimize disposal problems and waste, always specify the smallest practical quantities in laboratory experiments.
- 2. Chemicals should be purchased in the appropriate amounts in practical container sizes. Storage of chemicals over long periods should be avoided since this increases the hazards of chemical accidents and is wasteful.
- 3. When disposing chemicals, keep different classes of waste chemicals in a separate disposal containers. Incompatible chemicals spilled together on a bench or placed into the same disposal container can cause a violent chemical reaction.
- 4. Place non-hazardous waste in a wastepaper basket, separate from chemical wastes. If the paper is contaminated, such as paper towels used to clean up a spill, place the paper in a specially labeled, combustible waste container with a self-closing lid. The combustible waste should be treated as chemical waste, and should be emptied daily.
- 5. Broken glass and glassware should be place in designated sharp waste container. Place broken plastic apparatus in a marked waste container different from the broken glass container. Broken mercury thermometers and manometers may contain mercury in the fragments. Dispose as waste mercury.
- 6. For discarded and unused chemicals, place each container of solid and liquid chemicals in its own specially marked container, based on hazard class compatibility. Close these containers after each use. Chemicals may be put down the drain only if the laboratory supervisor has approved this method of disposal, and the chemical is determined to be non-hazardous and non-polluting. Solutions of acids or bases should be neutralized before disposal. Do not pour water-insoluble chemicals into the sink or down a drain. Chemicals pour into the sink can damage plumbing and sewer systems, and can cause environmental damage. If it happens accidentally, notify the laboratory supervisor.
- c. List of Incompatible Chemicals (see Table B1)

Chemical	Incompatible with
Acetic Acid	Chromic acid, nitric acid, hydroxyl compounds, ethylene
	glycol, perchloric acid, peroxides, permanganates
Acetylene	Chlorine, bromine, copper, fluorine, silver, mercury

Table B1. List of laboratory chemicals and their incompatibilities.

Chemical	Incompatible with
Acetone	Conc. nitric acid and sulfuric acid mixtures
Ammonia gas (anhydrous)	Mercury (e.g. in manometers), chlorine, calcium hypochlorite, iodine, bromine, hydrofluoric acid (anhydrous)
Ammonium nitrate	Acids, powdered metals, flammable liquids, chlorate nitrates, sulfur, finely divided organic combustibl materials
Aniline	Nitric Acid, hydrogen peroxide
Arsenical materials	Any reducing agent
Azides	Acids
Bromine	See chlorine
Calcium oxide	Water
Carbon (activated)	Calcium hypochlorite, all oxidizing agents
Chlorates	Ammonium salts, finely divided organic or combustible materials
Chromic acid and chromium trioxide	Acetic acid, naphthalene, camphor, glycerol, alcoho flammable liquids in general
Chlorine	Ammonia, acetylene, butadiene, methane, propane (conterpetroleum gases), hydrogen, benzene, finely divide metals, turpentine
Chlorine dioxide	Ammonia, methane, phosphine, hydrogen sulfide
Copper metal	Acetylene, hydrogen peroxide
Cumene hydroperoxide	Acids (organic or inorganic)
Cyanides	Acids
Flammable liquids	Ammonium nitrate, chromic acid, hydrogen peroxiden nitric acids sodium peroxides, halogens
Fluorine	All other chemicals
Hydrocarbons (such as butane, propane, benzene)	Fluorine, Chlorine, bromine, acid, sodium peroxide
Hydrocyanic acid	Nitric acid, alkali
Hydrofluoric acid	Ammonia (aqueous or anhydrous)
Hydrogen sulfide	Fuming nitric acid, oxidizing gases
Hydrochlorites	Acids, activated carbon
Iodine	Acetylene, ammonia (aqueous or anhydrous), hydrogen
Mercury	Acetylene, fulminic acid, ammonia
Metals of Groups I and II and powdered Group III	Water, carbon tetrachloride, halogens
metals Nitrites	Acids
Nitric acid (concentrated)	Acetic acid, aniline, chromic acid, hydrocyanic acid, hydroge
while acter (concentrated)	sulfide, flammable liquids and gases, copper, brass, any heav metals
Nitroparaffins	Inorganic bases, amines
Oxalic acid	Silver, mercury
Oxygen	Oils, grease, hydrogen, flammable liquids
Perchloric acid	Acetic anhydride, bismuth and its alloy, alcohol, pape wood, grease, oils
Peroxides, organic	Acids (organic or mineral), avoid friction, store cold
Phosphorous (white)	Air, oxygen, alkalis, reducing agents

Table B1. continued

Chemical	Incompatible with
Potassium metal	Carbon tetrachloride, carbon dioxide, water
Potassium chlorate	Sulfuric and other acids
Potassium perchlorate (see	Sulfuric and other acids
also chlorates)	
Potassium permanganate	Glycerol, ethylene glycol, benzaldehyde, sulfuric acid
Selenides	Reducing agents
Silver metal	Acetylene, oxalic acid, tartaric acid, ammonium compounds, fulminic acid
Sodium metal	Carbon tetrachloride, carbon dioxide, water
Sodium nitrite	Ammonium nitrate and other ammonium salts
Sodium peroxide	Ethyl or methyl alcohol, glacial acetic acid, acetic anhydride, benzaldehyde, carbon disulfide, glycerin, ethylene glycol, ethyl acetate, furfural
Sulfides	Acids

Table B1. continued