#### **1. INTRODUCTION**

Debre Berhan University has started offering three year undergraduate programs in chemistry for the last ten years. The department launched a post-graduate MSc program in area of specialization organic chemistry. This was a turning point in the history of the department and a significant step forward towards fulfilling the country's needs for high-level qualified chemists. The members of the department have been diligently working over the years to fulfill the expected aims and objectives of the country at large and the university in particular. From time to time, the department has been updating the curricula and organizing the academic schedules to cater to the needs of professionals, and research scholars to work in various industries and research laboratories and to teach in educational institutions in the country.

The practice of analytical chemistry has now become an integral and essential component in many diverse spheres such as Food and Beverage industry, Pharmaceutical industry, Chemical synthesizing and producing industries, Environmental control, Electrochemical technology, Agriculture, etc. Many of the underlying principles of Analytical Chemistry can be seen routinely in analysis in many areas such as quality control, research and development work, manufacturing processes, and in industry, university, and other research laboratories.

#### **2. RATIONALE**

The rapid expansion and development in higher education, agriculture and industrialization sections throughout the country because of increase in population growth, there is increasing demand for fuel, pesticides, fertilizers, industrial chemicals, pharmaceuticals, processed food, textiles and similar indispensable products, has been associated with society's desire to enhance the quality of life. As a matter of fact industrialization offering commodities and services to the public to meet such demands which has been resulted in waste products, which are released into the environment through wastewaters, gaseous emissions, and solid residues, leading to environmental pollution and a deterioration of natural resources. It has attained the stage that the earth's in-built ecosystem could no longer dilute, decompose and recycle the waste products. So at this stage knowing the source of environmental pollution and taking waste treatment measure

is mandatory. Thus to control the quality of the product and environmental pollution equipping with knowledge of analytical chemistry is necessary.

The post-graduate, Analytical chemistry program in the Department of chemistry will serve to upgrade the skills of scores of BSc/BED chemists from higher institutions of learning and other governmental and non-governmental organizations. The MSc. program, which will be launched, will help to produce man power capable of shouldering teaching and research position technical support expertise in universities, industries and various socioeconomic sector of the country such as sugar, alcoholic beverages, soap and detergent, leather, textile industries etc as quality control expert or production manager.

The opening of the program will help to retain academic staff members by creating conducive environment for research work which is essential for academic carrier and professional satisfaction

#### 2.1 Need Assessment Results

The department of chemistry did need assessment in high School, preparatory school, in industries such as brewery, food and research center about launching of the program and its importance. The result of the assessment showed that all agree the opening of analytical chemistry with high interest to attend the program. There will be also research collaboration, material exchange/support, training activities with the department.

### 2.2 Opportunities

There are many situations which is important in particular for chemistry department in general for university to provide education opportunity for high school, preparatory school, higher education institute, industry, research center worker to upgrade their knowledge. The various industries also serve as sources of research problem and instruments. The other point is having a potential research area which is Ankober herbal project and the university waste treatment plant. The natural product project have significant role to do research on the herbal medicinal plant extracts and develop further project internationally and nationally. The other area is the water treatment plant which is essential to enhance the quality of water through the research work.

# 2.3. Resource Available 2.3.1 Staff Profile

# Academic staff members on duty

No	Name	Academic rank	Specialization
1	Tesfaye Demse (PhD)	Assistant professor	Physical chemistry
2	Abebe Tedla (PhD)	Assistant professor	Organic chemistry
3	Amare Ayalew (PhD)	Assistant professor	Analytical chemistry
4	Adanech Alemu	Lecturer	Analytical chemistry
5	Teshome Asefa	Lecturer	Physical chemistry
6	Haftu G/tsaddik	Lecturer	Physical chemistry
7	Abayneh Kassahun	Lecturer	Organic chemistry
8	Solomon Mulawu	Lecturer	Physical chemistry
9	Belachewu Kebede	Lecturer	Inorganic chemistry
10	Getu Kasegn	Lecturer	Physical chemistry
11	Giday G/egziabhere	Lecturer	Organic chemistry
12	Yosef Shiferawu	Lecturer	Analytical chemistry
13	Abdisa Gebisa	Lecturer	Inorganic chemistry
14	Gezu Feleke	Lecturer	Organic chemistry
15	Mekdes Gerawork	Lecturer	Inorganic chemistry
16	Rediate Fikadu	Graduate assistant	-

## Technical assistant on duty

No	Name	Academic rank	Specialization
1	Yeneneh Getachew	Technical assistant	-
2	Gebru Nigussie	Technical assistant	-
3	Terefe Gebremariyame	Technical assistant	-
4	Menelik Ayalew	Technical assistant	-

No	Name	Academic rank	Specialization
1	Bizuayehu Tadesse	lecturer	Analytical chemistry
2	Yosef Alemayehu	lecturer	Environmental chemistry
3	Minbale Gashu	lecturer	Organic chemistry
4	Eskinder teklu	lecturer	Analytical chemistry
5	Alemnewu Birhanu	lecturer	Environmental chemistry
6	Asfawu Negash	lecturer	Physical chemistry
7	Kalayou Hiluf	lecturer	Analytical chemistry
8	Neway Belachewu	lecturer	Inorganic chemistry
9	Balkewu Zewug	lecturer	Analytical chemistry
10	Belete Tewabe	lecturer	Organic chemistry
11	Liboro Hinditu	lecturer	Inorganic chemistry
12	Jemal Mahamed	lecturer	Physical chemistry

### Academic staffs on study leave (PhD program)

### **2.3.2 Laboratory Facilities**

The chemistry department needs modern instruments for analysis and synthesis of chemicals (modern chemical research), advance training in modern areas of chemistry and other related disciplines. Some of the instrumentation facilities available in the department are:

- UV-VIS spectrophotometer,
- Atomic Absorption Spectroscopy (AAS)
- Microprocessor Based Conductivity/TDS Meter,
- pH Meter,
- Melting Point Apparatus etc.
- Suction Filtration pump
- Bomb Calorimeter etc.
- Soxelet

Besides, the department of chemistry is in the position to get instruments, which are very essential for the successful running of the program:

- UV-VIS spectrophotometers,
- Fourier Transform Infrared Spectrometer (FTIR)
- High Performance Liquid Chromatography (HPLC)
- Gas Chromatography (GC)
- Flame Photometer (FP)
- Cyclic voltammeter
- Thermo-gravimetric Analyzer (TGA)
- Acid decomposition/digestion vessels
- Scanning electron microscope
- X-ray diffractometer

# 3. RESEARCH-BASED MSc. PROGRAM

# 3.1 Objectives to be achieved by the Analytical chemistry MSc. program

- To have skilled manpower of well-trained chemists, capable of taking up positions in various socio-economic sectors of the country
- To build research capabilities as required by the national development and academic needs
- To develop capability for the provision of consultancy and technical service as well as short term specialized training to both public and private sectors
- To advance frontiers of knowledge in the area of chemical sciences
- To disseminate knowledge on chemistry and related areas through active participation in related professional activities such as publications, national and international symposiums
- To develop capabilities for the provision of consultancy and technical services as well as short term specialized training to both public and private sectors
- To support other higher learning education, such as Biology, Biotechnology, Chemical Engineering and other basic sciences through the provision of supportive courses and to undertake research activities
- To stimulate scientific curiosity and general intellectual objectives aimed at producing matured and conscious citizens

- To conduct collaborative research in the areas of natural products with various departments within the University and other institutions
- To fulfil teaching staff required in our university and to those recently opened universities

## **3.2 Graduate Profile**

A Graduate with M.Sc. Degree in Analytical Chemistry after successful completion of intensive M.Sc. training in the Department of Chemistry should be able to:

- Conduct research independently and in collaboration with others to meet the societal needs
- Serve as instructors in the field of Analytical chemistry and related areas at higher education institutions
- Manage and/or supervise processes and operations in various sectors of the economy
- Demonstrate environmentally conscious attitude, behave as a responsible citizen and demonstrate professional ethics
- Consult the concerned bodies in matters related to chemical knowledge
- Adapt and introduce new scientific developments including scientific instruments and their optimized utilization

## **3.3** Admission Requirements

Applicants are admitted into the MSc program in Analytical Chemistry once a year. And they should meet the following requirements:

- Applicants must have BSc/B.ED degree in chemistry or equivalent from any recognized university/College.
- ✤ Applicants must successfully pass an entrance examination of the department.
- ✤ Applicants must meet the general admission policies of the University.

### 3. 4 Graduation Requirements

Candidates are eligible for graduation upon successful completion of all stated courses and thesis work. They should fulfill the requirements indicated below. Candidates:

- should score cumulative Grade point average (GPA): 3.00 and above with no F and D grades in any course
- should successfully defend thesis and score Satisfactory and Above
- If a student has a grade of C<sup>+</sup> or C in more than one course, he/she is subjected to repeat the course
- Successful completion of all the specified courses minimum credit hour requirement is
  36

### **3.5 Degree Nomenclature**

The Degree of Master of Science in Chemistry (Analytical) በአማርኛ: የሳይንስ ማስተር ዲግሪ በኬሚስትሪ (አናሳይቲካል)

## 3.6 Field of Study

The M.Sc. program is conducted in research-based in Analytical chemistry. The program consists of a set of core courses accounting for a total of 30 Cr. Hrs and additional 6 credit hours of M.Sc. thesis research. Thus, the minimum requirement of courses and thesis research shall be 36 credit hours. The selection of students to the stream shall be decided by the department graduate committee, taking student's choice in to consideration.

### 3.7 Duration of Study

The duration of study is 2 years (4 semesters) for regular program, 3 years (8 semesters) for extension programs and 4 years (4 summers) for summer program. The program can be extended for a semester (s) under special case with the recommendation of research supervisor with the

consent of department graduate committee (DGC) and approved by the graduate program academic commission (GPAC).

# **3.8** Assignment of Course Code

All courses given by the Department of Chemistry start with a code Chem. followed by a threedigit number. The first digit indicates the level of the course (5 for first year and 6 for second year of the graduate course).

- 1 Inorganic Chemistry,
- 2 Analytical Chemistry
- 3 Physical Chemistry,
- 4 Organic Chemistry,
- 5 Introduction to Research methods and
- 9 Seminar, research and related courses.

The 3rd digit indicates the semester of the course offered:

- ODD numbers are offered during the first semester
- EVEN numbers are offered during the second semester.

### 4. Course delivery methods

• All courses in each program will be delivered in parallel but if there are some special cases that block teaching is necessary, we can apply it.

• Teaching methodology shall be student – centered which includes:

i) Course work

- Lectures
- Presentations/term paper
- Using LCD and ICT facilities.
- Others...

ii) Laboratory work

- Demonstration method
- Individual experiment
- Group experiment

iii) Thesis work

• Thesis should be done individually by candidate

# 4.1. Mode of assessment

Generally, assessment and evaluation of students' work in this program is based on the assessment policy of the University. Alternative (Authentic) continuous assessment principles and techniques will guide assessment and evaluation activities of the program. At least 50 % of the assessment will be based on continuous assessment. More specifically, the following assessment techniques will be given much attention.

- A Individual work
- $\cancel{P}$  Individual and Group presentations
- $\cancel{P}$  Test/mid semester examination and final examination for course work
- For practical courses laboratory reports, field reports, practical examinations, and written examinations.
- Feedback: regular feedback from students

# 4.1.1 Course Policy

For course work and practical courses, if a candidate miss more than 15% of the class attendance he/she will not sit for final exams. All students are expected to abide by the code of conduct of the university Academic legislation throughout this course. Academic dishonesty, including cheating, fabrication, and plagiarism will not be tolerated and will be reported to concerned bodies for action.

## 4.1.2. Grading System

The grading system of the program will be based on the University's legislation and is given as follows

RawMark	Corresponding Fixed	Corresponding	Status Description
Interval-[100 %]	Number Grade	LetterGrade	
[90,100]	4.0	$A^+$	Excellent
[85, 90)	4.0	А	
[80, 85)	3.75	A	
[75, 80)	3.5	$B^+$	VeryGood
[70, 75)	3.0	В	
[65, 70)	2.75	B	Good
[60, 65)	2.5	$C^+$	
[50, 60)	2.0	С	Satisfactory
[45, 50)	1.75	C -	Unsatisfactory
[40,45)	1.0	D	Very Poor
[30,40)	0	Fx	*Fail

# 4.1.3. Thesis Evaluation and Rating

Generally, the thesis evaluation of students' work in this program is based on the legislation of the University.

- Mathematical A thesis is based on original research work.
- Thesis evaluation includes both oral presentation and the quality of thesis work
- Evaluation should be done by the internal and external examiners.
- A Thesis that is defended and accepted may be rated as "Excellent", "Very Good", "Good" or "Satisfactory".
- A candidate must obtain at least "Satisfactory" in his/her Thesis.
- Main A rejected thesis shall be rated "Fail".

Rank	Percent (%)
Excellent	$\geq 85$
Very Good	$75 \le X < 85$
Good	$60 \le X < 75$
Satisfactory	$50 \le X < 60$
Fail	<50

The grading scales of each rank of the thesis are as follows:

# 5. Courses to be taken :

S.No.	Course code	Title of courses	Cr.hrs	ECTS
1	Chem.511	Advanced Inorganic Chemistry	3	5
2	Chem.531	Advanced Physical Chemistry	3	5
3	Chem.541	Advanced Organic Chemistry	3	5
5	Chem.552	Introduction to Research Methods	2	3
6	Chem.521	Advanced Analytical Techniques	3	5
7	Chem.522	Advanced Practical Analytical techniques	2	3
8	Chem.528	Chemometrics, Statistics and Quality	3	5
		Assurance in analytical Chemistry		
9	Chem.526	Separation Science	2	3
10	Chem.592	Seminar I	1	2
	Chem.691	Seminar II	1	2
11	Chem.621	Analytical Applications of Complex	3	5
		Equilibria and Modern Extraction Techniques		
12	Chem.624	Electroanalytical Chemistry	2	3
14	Chem.523	Special Topics in Analytical Chemistry	2	3
16	Chem.598	Thesis	6	10
	Total	Cr. hrs	36	59

# 5.1 Course Breakdown for Regular Program

# Year I/ Semester I

Course Code	Title of courses	Cr. hrs	ECTS
Chem. 521	Advanced Analytical Techniques	3	5
Chem.511	Advanced Inorganic Chemistry	3	5
Chem.541	Advanced Organic Chemistry	3	5
Chem.531	Advanced Physical Chemistry	3	5
Semester Total		12	20

# Year I/Semester II

Course Code	Title of courses	Cr. hrs	ECTS
Chem. 552	Introduction to Research Methods	2	3
Chem. 522	Advanced Practical Analytical Techniques	2	3
Chem. 524	Electroanalytical Chemistry	2	3
Chem. 526	Separation Science	2	3
Chem. 528	Chemometrics, Statistics and Quality Assurance in analytical Chemistry	3	5
Chem. 592	Seminar I	1	2
Semester Total		12	19

## Year II /Semester I

Course Code	Title of courses	Cr. Hrs	ECTS
Chem. 621	Analytical Applications of Complex Equilibria	3	5
	and Modern Extraction Techniques		
Chem. 623	Special Topics in Analytical Chemistry I	2	3
	(elective course)		
Chem. 691	Seminar II	1	2
Chem. 698	Thesis	-	-
Semester Total		6	10

# Year II /Semester II

Course Code	Title of courses	Cr. hrs	ECTS
Chem. 698	Thesis	6	10
Semester Total		6	10

# 5.2 Course breakdown for summer program

### Summer- I

Course code	Title of courses	Cr. hrs	ECTS
Chem. 511	Advanced Inorganic Chemistry	3	5
Chem. 531	Advanced Physical Chemistry	3	5
Chem. 541	Advanced Organic Chemistry	3	5
Semester Total		9	15

# **Distance-I**

Course code	Title of course	Cr. Hrs	ECTS
Chem. 552	Introduction to Research methods	2	3
Semester Total		2	3

### Summer – II

Course code	Title of courses	Cr. Hrs	ECTS
Chem. 521	Advanced Analytical Techniques	3	5
Chem.522	Advanced Practical Analytical techniques	2	3
Chem.526	Separation Science	2	3
Chem.524	Electroanalytical Chemistry	2	3
Semester Tota	al	9	14

## **Distance-2**

Course code	Title of courses	Cr. hrs	ECTS
Chem. 592	Seminar I	1	2
Semester Total		1	2

Course code	Title of courses	Cr. Hrs	ECTS
Chem 528	Chemometrics and Quality	3	5
	Assurance in analytical Chemistry		
Chem 621	Analytical Applications of	3	5
	Complex Equilibria and Modern		
	Extraction Techniques		
Chem 623	Special Topics in Analytical	2	3
	Chemistry (elective course)		
Semester Tota	Semester Total		13

# Summer-III

# **Distance III**

Course code	Title of courses	Cr. hrs	ECTS	
Chem. 691	Seminar II	1	2	
Chem. 698	Thesis	-	-	
Semester Total	·	1	2	

# Summer –IV

Course code	Title of course	Cr. Hrs	ECTS
Chem. 698	Thesis	6	10
Semester Total		6	10

# 5.3 Course breakdown for extension program

# Year I / Semester I

Course code	Title of courses	Cr. hrs	ECTS
Chem. 511	Advanced Inorganic Chemistry	3	5
Chem. 541	Advanced Organic Chemistry	3	5
Semester Total		6	10

## Year I / Semester II

Course code	Title of courses	Cr. hrs	ECTS
Chem. 521	Advanced Analytical Techniques	3	5
Chem. 531	Advanced Physical Chemistry	3	5
Semester Total	·	6	10

# Year I / Semester III

Course code	Title of courses	Cr. hrs	ECTS
Chem.522	Advanced Practical Analytical techniques	2	3
Chem.528	Chemometrics, Statistics and Quality Assurance in analytical Chemistry	3	5
Semester Total		5	8

## Year II / Semester I

Course code	Title of courses	Cr. hrs	ECTS
Chem.526	Separation Science	2	3
Chem. 552	Introduction to Research methods	2	3
Chem. 592	Seminar I	1	2
Semester Total		5	8

Course code	Title of courses	Cr. hrs	ECTS
Chem.524	Electroanalytical Chemistry	2	3
Chem.621	Analytical Applications of Complex Equilibria and Modern Extraction Techniques	3	5
Semester Total		5	8

# Year II/ Semester II

# Year II/ Semester III

Course code	Title of courses	Cr. hrs	ECTS
Chem.623	Special Topics in Analytical Chemistry	2	3
Chem. 691	Seminar II	1	2
Semester Total	·	3	5

# Year III/ Semester I

Course code	Title of courses	Cr. hrs	ECTS
Chem.698	Thesis	-	-
Semester Total		-	-

## Year III/ Semester II

Course code	Title of courses	Cr. hrs	ECTS
Chem.698	Thesis	6	10
Semester Total		6	10

### 6. Course Description and Outlines

Course Title: Advanced Inorganic Chemistry Course Code: Chem.511 CR. Hrs: 3 ECTS: 5 Status of the Course: Compulsory Pre-requisites: -

### **Course Description**

Crystal field and molecular orbital theories: Salient features of metal-ligand bonding as elucidated by Crystal field theory and molecular orbital theory; geometries, magnetic properties, term splitting, strong and weak field consequences; symmetry and group theoretical considerations of sigma and pi bonding. Solid state: Types of solids; Fast ion conductors, Super conductors;

**Course Objectives** Upon completion of this course the students will gain familiarity with the frontier areas of inorganic chemistry. They will

• Gain knowledge of structure and bonding in a variety of inorganic compounds, with particular reference to metal complexes from different theories approach

- Acquire detailed understanding of the major theories of bonding in metal complexes
- Discuss the classification and applications of various solid state materials
- Define and identify super conductors and appreciate their application

## **Course Content**

- 1. Crystal Field Theory
- 1.1. Splitting of *d*-orbitals in various geometries
- 1.2. Factor influencing crystal field splitting-CFSE
- 1.3. Magnetic properties-High spin, low spin crossover.
- 1.4. Thermodynamic aspects
- 1.5. LS coupling-splitting of terms in weak and strong fields Limitations

2. Molecular Orbital Theory: Symmetry classification of metal and ligand orbitals in cubic and non-cubic environments Construction of MOED for *O*h, *T*d and *D*4h complexes with sigma and  $\pi$ -bonding

- 3. Activation of small molecules:
- 3.1. Ligational aspects of CO, NO, O<sub>2</sub>, H<sub>2</sub>
- 3.2. Structures and types of bonding.
- 3.3. Spectral and magnetic properties
- 4. Cluster Compounds
- 4.1. Classification of Boranes-Wade's rules
- 4.2. Types of lower halide metal clusters
- 4.3. Bonding in dinuclear and octahedral metal clusters Low and high nuclearity metal

carbonyls-electron counting schemes

- 4.4. Concept of isolobality
- 4.5. Applications of metal clusters
- 5. Solid State
- 5.1. Classification of Solids
- 5.2. Liquid crystals
- 5.3. Spinels, pyrochlores, bronzes and silicates
- 5.4. Fullerenes and nano materials
- 5.5. Fast ion conductors and Super conductors
- 5.6. Stoichiometric and non-stoichiometric defects
- 5.7. L'Hopital's rule and indeterminate forms
- 5.8. Graph sketching

## **Mode of Delivery**

- Individual and group presentation
- Group work
- Project work

### Assessment

• Mid exam	30%.
• Individual assignment and Presentation	20%
• Final Exam	50%
• Total	.100%

## **Text books**

 F.A. Cotton, G. Wilkinson, CA. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Ed., Wiley Interscience, New York, 1999.

# References

1. B.E. Douglas, D.H. Mcdaniels and J. Alexander, Concepts and models in Inorganic Chemistry, Wiley, New York, 1983.

2. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry, Principles of structure and reactivity,4th Ed., Harper & Row, Cambridge, 1993.

3. K.F. Purcell and J. C. Kotz, Inorganic Chemistry, Saunders, Philadelphia, 1977.

4. C.E. Housecroft and A.G. Sharpe, Inorganic Chemistry, Prentice Hall, Harlow, 2001.

5. M. Gerloch and E.C. Costable, Transition Metal Chemistry: The valence shell in *d*-block Chemistry, VCH publishers, Weinheim, 1994.

6. B.N. Figgis, Ligand Fields, Wiley, New York, 1966.

7. A.R. West, Solid State Chemistry and its applications, Wiley, New York, 1984.

8. C.N.R. Rao and J. Gopalakishnan, New directions in solid state Chemistry, Dekker, New York, 1986.

9. N.N. Greenwood and A. Earnshaw, Chemistry of Elements, Butterworth-Heinemnn, Oxford, 1997.

10. M.N. Hughes, The Inorganic Chemistry of Biological Processes, 2nd Ed., Wiley, Chichester, 1981.

11. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3rd Ed., Oxford University Press, Oxford, 1999.

Course Title: Advanced Physical Chemistry

Course Code: Chem. 531 Cr.hrs: 3 ECTS: 5

Status of the Course: Compulsory

**Pre-requisites:-**

**Course Description** Introduction to Quantum Theory, Fall of classical mechanics and down of quantum mechanics, Operators, Angular momentum in Quantum mechanics, Solutions of Schrödinger Equation for Simple Systems, Atomic Structure, Approximation Methods in

Quantum mechanics, Molecular Structure, Molecular Spectroscopy, Molecular Term Symbols, Elementary Chemical Kinetics Aspects, Reaction order determination, Experimental Methods of Chemical Kinetics, Temperature Effect on Reaction Rate, Complex Reactions, Theories of Reaction Rate, Kinetics of Some Special Reactions, Kinetics of Catalyzed Reactions, and Fast Reactions.

Course Objectives Upon completion of this course the students will be able to:

• Understand the fundamentals of quantum mechanics and to apply quantum mechanics to simple to complex systems

- Use the Schrodinger Equations for computing Chemical problems
- To learn quantum mechanical principles and their application to atoms and molecules
- The student will be able to understand the basic concepts of chemical kinetics
- Determine the reaction rate theories and rate laws
- Deduce the reaction mechanism

## **Course Content**

- 1. Quantum Chemistry
- 1.1 Historical back ground of quantum mechanics
- 1.2 Blackbody-Radiation (Mathematical Approach)
- 1.3 The Wave Nature of Matter
- 1.4. Heisenberg's Uncertainty Relation
- 1.5. Photoelectric effect
- 2. The time dependent and time independent Schrodinger equation
- 3. Operators
- 4. Eigen values and Eigen functions
- 5. Angular Momentum in the Quantum Mechanics
- 6. Quantum mechanics of simple systems
- 6.1.Particle in a one dimensional box
- 6.2.Particle on a ring
- 6.3.Particle on a sphere
- 6.4.Harmonic oscillator

- 7. Atomic structure
- 7.1. The Hydrogen Atom and Similar Atoms
- 7.2.Pauli Principle
- 7.3. The Hydrogen Molecule Ion and Similar Systems
- 8. Approximation methods in quantum mechanics
- 8.1.The variation method
- 8.2. Perturbation theory
- 8.3. Hartee and Hartee-fock self -consistent field theories
- 9. Molecular Structure
- 9.1. The Born-Oppenheimer Approximation
- 9.2. The Chemical Bond 9.2.1. Molecular Orbital Theory
- 9.2.2. Valence Bond Theory
- 9.2.3. Hybridization
- 9.2.4. The Huckel Molecular Orbital Theory
- 9.3. Molecular Term Symbols
- 9.4. Molecular Spectroscopy
- 9.4.1. General Features of Spectroscopy
- 9.4.2. Electronic Transitions
- 9.4.3. Pure Rotational Transitions
- 9.4.4. Vibrational Transitions
- 10. Chemical Kinetics
- 10.1. Reaction rates and rate laws
- 10.2. Simple kinetic forms
- 10.3. Steady state approximation
- 10.4. Deduction of reaction mechanism
- 10.5. Reaction rate theories and reaction energetics
- 10.6. Temperature dependence of rate constant
- 10.7. Activation parameters
- 10.8. Kinetics and thermodynamics
- 10.9. Collision theory
- 10.10. Gaseous reaction

- 10.10.1.Unimolecular, bimolecular and trimolecular reactions
- 10.11. Reactions on surfaces
- 10.11.1.Unimolecular and bimolecular surface reactions
- 10.12. Complex reactions
- 10.12.1. Linear and branched chain reactions
- 10.12.2.Oscilating chemical reactions
- 10.12.3.Catalytic reactions
- 10.12.3.1. Acid base catalysis
- 10.12.3.2. Enzyme catalysis
- 10.13. Kinetics of fast reactions
- 10.13.1.Relaxation method
- 10.13.2.Relaxation spectrometry
- 10.13.3.Flow method
- 10.13.4.Shock method

### **Mode of Delivery**

- A Lecture
- $\cancel{}$  assignments
- $\cancel{P}$  Demonstration of experimental facts

### Assessment

• Total	100%
• Final exam	50%
Individual Assignment	20%
• Mid exam	30%

## References

1. I. N. Levine, Quantum Chemistry, 5th Ed., Prentice-Hall, New Jersey, 2000.

2. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 3rd Ed., Oxford Univ. Press, USA, 1997.

3. D.A. McQuarrie and J.D. Simon, Quantum Chemistry: A Molecular Approach, 5th Ed., Viva Books Private Limited, 2006.

4. J. E. House, Fundamentals of Quantum Chemistry, 2nd Ed., Academic Press, California, USA, 2004.

5. A. Szabo and N.S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, 1996.

J. E. House, Principles of Chemical Kinetics, 2nd Ed., Academic Press, San Diego, USA, 2007.

7. M. Mortimer, P. Taylor, The molecular World: Chemical Kinetics and Mechanisms, R.S.C. Cambridge, UK, 2002.

8. F. Daniels, Chemical Kinetics, Cornell University Press, New York, USA, 1938.

Course Title: Advanced Organic Chemistry I Course Code: Chem.541 Cr.Hrs: 3 ECTS: 5 Status of the Course: Compulsory Pre-requisites: -

#### **Course Description**

This course is a comprehensive survey of organic chemistry with emphasis on stereochemistry and important synthetic reactions. It provides a broad view of stereochemical principles and conformational analysis. It also aims to improve students' understanding of organic reaction mechanisms and reactivity. The objective of this course therefore is to study how structure (bonding, stereochemistry, conformation, energy, etc.) determines the reactivity of a given molecule: what type of reaction is a given molecule likely to undergo? What is the mechanism of the reaction and how this mechanism related to the structure of the molecule, how the structures of organic compounds are related to their reactivity? Thus, the following topics will be covered in detail; chemical bonding and molecular structure, stereochemical principles, conformational, steric and stereoelectronic effects, nucleophilic substitution, polar addition and elimination reactions. The course emphasizes selectivity in organic chemistry and the underlying principles behind chemoselectivity, enantioselectivity, regioselectivity and diastereoselectivity are discussed.

Course Objectives After completion of this course, the students will be able to:

- Appreciate that the conformation of a molecule dictates how it will react and Appreciate the reaction selectivity such as, chemoselectivity, enatioselectivity, regioselectivity and diastereoselectivity in reaction pathways
- Understand the principal methods currently available to achieve the stereoselective and stereospecific synthesis of organic compounds and appreciate the challenge of synthesizing enantiopure compounds
- predict a reasonable mechanism for any type of organic reaction and suggest the most reasonable ways of forming a given organic molecule
- Predict the most likely reaction to a given molecule likely to undergo under a given set of conditions
- $\cancel{P}$  Suggest experimental methods to establish or reject a suggested mechanism
- Appreciate the utility of reactive intermediates such as carbanions, carbocations, carbenes and free radicals and understand the concept of reactivity with respect to intermediatesstereochemistry in organic reactions
- Suggest possible structures for intermediates

# **Course Content**

- 1. Chemical bonding and molecular structure: Description of molecular structure
- 1.1. Using valence bond concepts
- 1.2. Molecular orbital methods
- 2. Stereochemical principles: Configuration
- 2.1. R,S nomenclature of enantiomers
- 2.2. Iisomerism: constitutional isomers and stereoisomers
- 2.3. Optical activity
- 2.4. Chirality, stereogenic center
- 3. Stereochemical principles: Configuration
- 3.1. Enantiomeric and diastereomeric relationships
- 3.2. Molecules with more stereogenic centers
- 3.3. Hreo, erythro and meso compounds
- 3.4. Fischer projection formulas

- 3.5. D,L nomenclature of enantiomers
- 3.6. relative and absolute configuration
- 4. Stereochemical principles: Configuration
- 4.1. Stereochemistry of dynamic processes
- 4.2. Prochiral relationships
- 4.3. Stereoselective and Stereospecific Reactions
- 4.4. Separation of Enantiomeric Mixtures
- 5. Conformational, Steric and Stereo-electronic effects:
- 5.1. Effect of heteroatoms on conformational equilibria, anomeric effect
- 5.2. Conformational effects on reactivity
- 5.3. conformations of unsaturated systems
- 5.4. Reactivity of cyclohexanone
- 5.5. Reactivity of bicycle[3.3.1]nonan-9-one
- 5.6. Relationship between ring size and rate of cyclization reactions
- 5.7. Steric and electronic effects on reactivity,
- 5.8. Effect of reaction center hybridization on reactivity
- 5.9. Cram's Rule: reactivity of bicyclo[2.2.1]heptene and its 7,7-dimethyl derivative
- 6. Structural effects on stability and reactivity:
- 6.1. kinetic and thermodynamic effects
- 6.2. relationships between Thermodynamic Stability and Reaction Rates
- 6.3. electronic Substituent Effects on Reaction Intermediates
- 6.4. kinetic Isotope Effects
- 6.5. linear Free-Energy Relationships for Substituent Effects
- 7. Nucleophilic Substitution:
- 7.1. Mechanism of nucleophilic substitution,
- 7.2. Structural and solvent effects on reactivity,
- 7.3. Neighboring group participation,
- 8. Nucleophilic Substitution:
- 8.1. Structure and reactions of carbocations,
- 8.2. Synthetic applications of carbocations
- 8.3. Stereochemistry of substitution reactions

- 9. Polar addition and elimination reactions:
- 9.1. Addition of halides and hydrogen halides
- 9.2. Hydration, sulfenylation, selenylation
- 9.3. Addition reactions involving epoxides.
- 9.4. Electrophilic addition involving metal ions
- 9.5. Synthesis and reactions of alkylboranes
- 9.6. Addition of alkynes and allenes
- 9.7. Elimination reactions
- 9.8. The E2, E1 an E1cb Mechanisms
- 9.9. Stereochemistry of Elimination reactions
- 10. Reactions involving highly electron-deficient intermediates:
- 10.1. Carbocations
- 10.2. Carbenes
- 11. Reactions involving highly electron-deficient intermediates:
- 11.1. Nitrenes
- 11.2. Free-radicals

## Mode of delivery

- Lecture methods
- Questions and answers

### Assessment

• Mid exam	30%
• Presentation and Individual assignment	.20%
• Final Exam	50%
• Total	100%

### **Text Book**

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry **Part A**: Structure and Mechanism, Plenum Press, New York, 2001.

2. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part B: Reactions and Synthesis, Plenum Press, New York, 2001.

#### References

1. Stuart Warren, Organic Synthesis: The Disconnection Approach, Wiley, 1982.

2. M.B. Smith, Organic Synthesis, McGraw Hill, 2002.

3. S.B. Smith and J. March, March's Advanced Organic Chemistry: Reactions, Mechanism and Structure, Wiley, 2001.

4. R.B. Grossman, The Art of Writing Reasonable Organic Reaction Mechanisms Springer, 2002.

5. Clayden, Greeves, Warren and Wothers, Organic Chemistry Oxford, 2001.

6. Robert S. Atkinson, Stereoselective Synthesis, Wiley, New York.

7. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley, New York.

8. E. L. Eliel, S. H. Wilen and M.P. Doyle, Basic Organic Stereochemistry Wiley, New York.

9. J. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, Wiley.

10. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge, 1986.

11. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms Harcourt/ Academic Press, 2002.

Course Title: Advanced Analytical Techniques

### Course Code: Chem.521 Cr.Hrs: 3 ECTS: 5

Status of the Course: Compulsory

### **Pre-requisites: -**

### **Course Description**

The course is designed to make the students develop competency in basic and theoretical principles in advanced analytical techniques. The course will familiarize and allow the students to specialize with the basic principle and application of different instrumentations like atomic absorption, atomic emission, ultraviolet-visible and infrared spectroscopy (UV-Vis and IR); nuclear magnetic resonance spectroscopy (NMR); fluorescence and phosphorescence instrumentations;

Course Objectives Upon the successful completion of this course, students will be able to:

• Understand and explain the underlying theories in UV-Vis, infrared, nuclear magnetic resonance spectroscopy, and mass spectrometry

• Describe the characteristics vibrational transition, electronic transition, nuclear magnetic resonance, molecular ionization, molecular ions, fragment ions, molecular formula, structural formula

• Distinguish the factors and their effects in the position and shapes of absorption peaks in UV-Vis, IR, NMR (1H and 13C) mass spectra

• Interpret vibrational, electronic, 1H, 13C NMR, mass spectra

• Apply the theoretical knowledge in interpreting the spectra in qualitative and quantitative analytical applications

# **Course Content**

- 1. UV/Vis Spectroscopy
- 1.1. Introduction
- 1.2. Selection Rules
- 1.3. Factors Affecting Electronic Absorption Spectra
- 1.3.1. Solvent Effects (Solvatochromic Effects) Solvent Effects on Spectra of
- 1.3.1.1. Nonpolar Molecules
- 1.3.1.2. Solvent Effects on Spectra of Polar Molecules
- 1.3.2. Effects of Conjugation Length
- 1.3.3. Type of Substituent
- 1.4 Electronic Spectra of Conjugated Dienes and Polyenes
- 1.5 Electronic spectra of Carbonyls and Enones
- 1.6 Electronic Spectra of Aromatic Compounds
- 1.7 Instrumentation
- 1.8 Applications of electronic spectroscopy
- 2. Infra Red (Vibrational) Spectroscopy
- 2.1 Introduction
- 2.2 Theory
- 2.2.1 Diatomic Molecules: The Harmonic Oscillator
- 2.2.2 Characteristic Stretching Frequencies of Some Molecular Groups

- 2.2.3 Polyatomic Molecules: Degree of Freedom
- 2.3 Overtones and combination Frequencies
- 2.4 Selection Rules
- 2.5 Interpretation of Infrared Spectra
- 2.4 Instrumentation
- 2.5 Sample Handling Technique
- 2.5.1 Liquid Samples
- 2.5.2 Solid Samples
- 3. Raman Spectroscopy
- 3.1 Introduction
- 3.2 Rotational Raman spectra
- 3.3 Vibrational Raman Spectra
- 3.4 Polarization of light and Raman effect
- 3.5 Structure elucidation from combined Raman and IR spectroscopy
- 3.6 Applications in structure elucidation
- 4. Nuclear Magnetic Spectroscopy
- 4.1 1H Nuclear Magnetic Resonance Spectroscopy
- 4.1.1 Basic principles: The origin of NMR spectra and nuclear relaxation
- 4.1.2 Instrumentation and sample handling
- 4.1.3 Chemical shift, factors affecting chemical shift
- 4.1.4 Spin-spin coupling or spin-spin splitting
- 4.1.5 Protons on heteroatoms: O-H, N-H, S-H groups
- 4.1.6 Coupling of protons with other nuclei, 19F, 31P, 2H, and 13C
- 4.1.7 Chemical shift equivalence and magnetic equivalence
- 4.1.8 AMX, ABX, and ABC systems
- 4.1.9 Factors affecting coupling constants: Vicinal coupling, Geminal coupling

4.1.10 Simplification of complex spectra: Increased field strength, spin-spin decoupling, Nuclear overhauser effect

- 4.2 13C Nuclear Magnetic Resonance Spectroscopy
- 4.2.1 Introduction
- 4.2.2 Chemical classes and Chemical shift

- 4.2.3 Coupling and decoupling in 13C NMR spectra
- 4.2.4 Determining 13C signal multiplicity using DEPT
- 4.2.5 Shielding and characteristic chemical shifts in 13C NMR spectra
- 4.2.6 Exercises on NMR
- 5. Mass Spectrometry
- 5.1 Introduction

5.2 Instrumentation 5.2.1 Methods of Ionization: electron impact, chemical ionization, SIMS, Fast atom bombardment, Field ionization, ESI, APCI

5.2.2 Mass Analyzer: Single and double focusing spectrometers; TOF, FT, MS/MS

5.3 The mass spectrum: Multiply charged and metastable ions

- 5.4 Elemental composition
- 5.5 The molecular ion, the nitrogen rule

5.6 Basic mechanisms of ion fragmentation: The even electron rule, Stevenson's rule, Loss of largest alkyl, Stability of the product ion,  $\sigma$ -cleavage,  $\beta$ -cleavage,  $\gamma$ -cleavage, McLafferty rearrangement, Interpretation of mass spectra and applications Structure Elucidation by Joint Application of UV, IR, NMR, and MS 7. Atomic Absorption Spectroscopy

- 7.1 Principle of AAS
- 7.2 Sample atomization techniques
- 7.3 Instrumentation
- 7.4 Interferences in AAS
- 7.5 Application
- 8. Spectroscopy based on Emission 8.1 Molecular Photoluminescence Spectroscopy
- 8.1.1 Molecular Fluorescence and Phosphorescence Spectra
- 8.1.2 Instrumentation 8.1.3 Quantitative Applications Using Molecular Luminescence
- 8.2 Atomic emission Spectroscopy
- 8.2.1 Basic principle
- 8.2.2 Instrumentation
- 8.2.3 Application

### **Teaching method**

- Demonstration
- Lecture

#### **Mode of Assessment**

• Total	100%
• Final Exam	50%
• Individual Assignment	20%
• Mid exam	

### References

1. G. Gauglitz, and T. Vo-Dinh, Handbook of Spectroscopy, Wiley-VCH, Weinheim, 2003.

2. R.M. Silverstein, C.G. Bassler, and T.C. Morrill, Spectroscopic Identification of Organic Compounds, 5th Ed., John Willey, New York, 1992.

3. 3. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5th ed., McGraw-Hill, New York, 1987.

4. C.N.R. Rao, Ultraviolet and Visible Spectroscopy, 3rd ed., Butterworths, London, 1974.

5. J.B. Lambert, H.F. Shurvell, L. Verbit, R.G. Cooks, and G.H. Stout, Organic Structural Analysis, Macmillan, New York, 1976.

6. F.W. McLafferty, Interpretation of Mass Spectra, 3rd ed., University Science Books Mill Valley, California, 1980.

7. L.D. Field, S. Sternhell, and J.R. Kalman, "Organic Structures from Spectra", 2nd ed., John Wiley, Chichester, 1995.

8. D.C. Harris, Quantitative Chemical Analysis, 4th ed., Freeman & Co., New York, 1995.

 S. Kumar. Spectroscopy of Organic Compounds, Guru Nanak Dev University, Amritsar -143005, 2006 Course Title: Advanced Practical Analytical techniques

Course Code: Chem.522 Cr. Hrs: 2 ECTS: 3

Status of the Course: Compulsory

# **Pre-requisites:-**

**Course Description** Lab experiments include Cyclic Voltammetry and amperometry, Gas chromatography (GC), High Performance Liquid Chromatography (HPLC), Infrared Spectroscopy (IR), Nuclear Magnetic resonance Spectroscopy (NMR), Ultraviolet spectroscopy (UV), Atomic absorption spectroscopy (AAS), etc. Experiments in Advanced Sample preparation and analysis methods will be designed. The students will be required to select optimized analysis method(s), including instrumentation(s), based on the sensitivity, selectivity, and cost and time efficiency

Course Objectives Upon the successful completion of this course, students will be able to:

• Apply various spectroscopic, chromatographic and electro-analytical techniques for qualitative identification and quantification of chemical substances

• Learn specific analytical techniques paramount for chemical analysis

• Learn to work safely in the laboratory

Get hands on practice on different analytical techniques and practical experience in the interpretation of analytical data from different instruments

• Learn how to write scientific laboratory reports, with special emphasis in data presentation and interpretation of the results.

# **Course Content**

**Experiment 1:** UV-Vis experiment (the effect of solvents on λmax shift) **Experiment 2:** UV-Vis experiment on the effect of substituent's and conjugation length on λmax and εmax **Experiment 3:** Infra Red spectroscopy experiment on liquid samples **Experiment 4:** Infrared spectroscopy experiment on alkali- halide discs and mull **Experiment 5:** NMR **Experiment 6:** GC/FID **Experiment 7:** GC/MS **Experiment 8:** HPLC/UV **Experiment 9:** LC-MS **Experiment 10:** Cyclic voltammetry **Experiment 11:** Chronoamperometric **Experiment 12:** Atomic absorption experiment (Determination of trace metals from water sample) **Experiment 13:**  Atomic emission experiment (Determination of Na and/K from solid foods after dry or wet ashing the food samples)

## Assessment

laboratory report and attendance	.50%
• Final Exam	50%
• Total	100%

## **Reference:**

1. G. Gauglitz, and T. Vo-Dinh, Handbook of Spectroscopy, Wiley-VCH, Weinheim, 2003.

2. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5th ed., McGraw-Hill, New York, 1987.

3. L.D. Field, S. Sternhell, and J.R. Kalman, "Organic Structures from Spectra", 2nd ed., John Wiley, Chichester, 1995.

4. F.W. McLafferty, Interpretation of Mass Spectra, 3rd ed., University Science Books Mill Valley, California, 1980.

5. S. Kumar. Spectroscopy of Organic Compounds, Guru Nanak Dev University, Amritsar - 143005, 2006

6. D.C. Harris, Quantitative Chemical Analysis, 4th ed., Freeman & Co., New York, 1995.

7. C.N.R. Rao, Ultraviolet and Visible Spectroscopy, 3rd ed., Butterworths, London, 1974.

8. J.B. Lambert, H.F. Shurvell, L. Verbit, R.G. Cooks, and G.H. Stout, Organic Structural Analysis, Macmillan, New York, 1976.

9. R.M. Silverstein, C.G. Bassler, and T.C. Morrill, Spectroscopic Identification of Organic Compounds, 5th Ed., John Willey, New York, 1992.

Course Title: Electroanalytical Chemistry

Course Code: Chem.524 Cr.Hrs: 2 ECTS: 3

Status of the Course: Compulsory

**Pre-requisites:** 

**Course Description** Potentials, thermodynamics and electrode kinetics aspect of the electrode solution interface. Mass transfer by migration and diffusion. Fick's first and second laws of

diffusion. Potential step methods (chronoamperometry) at planar and spherical electrodes; current-potential characteristics for reversible, irreversible and quasi-reversible electrode processes; potential sweep methods: linear sweep and cyclic voltammetry for reversible, irreversible and quasi-reversible systems; polarography and pulse voltammetry: normal, differential, pulse and square wave voltammetry, current-potential characteristics for reversible, irreversible and quasi-reversible electrode processes; controlled current techniques: chronopotentiometry; hydrodynamic methods: theoretical treatment of convection systems, current-potential curves at a rotating disk electrode, rotating disc and rotating ring-disc electrodes; techniques based on concepts of impedance: ac polarography/voltammetry, Bulk electrodysis methods, Electrogravimetry; Coulometry; stripping analysis; modified electrodes.

Course Objectives Upon the successful completion of this course, students will be able to:

• define terms such as inner, outer and surface potentials, polarizable and non-polarizable interfaces, potential of zero charge, overpotential, charge transfer resistance, migration, diffusion, convection, mass transfer coefficient, reversible reaction, diffusion-controlled reaction, charge transfer controlled reaction, irreversible reaction, Diffusion layer model, diffusion layer thickness,

• state Fick's 1st and 2nd laws of diffusion, and solve the diffusion equations for given boundary and limiting conditions,

- Examine the electrode kinetic parameters from experiments using chronoamperometry,
- understand the factors affecting the diffusion current in dc polarography and the current potential relationship for an irreversible reaction in dc polarography

• derive expressions for peak half-width potential in differential pulse polarograhy / voltammetry,

• analyze current-potential data to determine the reversibility of a redox reaction,

• explain the principles behind anodic stripping analysis and the principles behind chemically modified electrodes,

### **Course Content**

1. The electrified interface

• Potential Difference across Electrified Interfaces; Inner, Outer and Surface Potentials;

- Structure of Electrified Interface
- 2. Electrode kinetics
- The general current overpotential equation; The Butler Volmer Equation;
- Limiting forms of the Butler Volmer equation The Tafel equation
- 3. Mass Transfer towards the electrode solution Interface
- · Linear diffusion to planar electrodes; Convection; Fick's second law
- 4. Chronoamperometry

Reversible reactions – the Cottrell Equation; Irreversible reactions; Quasi-reversible reactions; Reversal technique; Chronocoulometry;

- 5. Chronopotentiometry
- Reversible reactions the Sand Equation; Irreversible reactions; Reversal technique
- 6. cyclic voltametry, dc polarography; Normal pulse polarography / voltammetry
- 7. Differential pulse polarography / voltammetry; Square Wave Voltammet
- 8. Impedance Techniques
- AC voltammetry /AC Polarography
- 9. Hydrodynamic Voltammetry

General Mass Transfer Equation - Nernst - Planck equation; Rotating Disc Electrode - Levich

equation; Reversible reactions; Irreversible reactions; quasi-reversible reactions

- 10. Bulk Electrolysis Methods
- Extent of Reaction,
- Current Efficiency;
- Controlled Potential Methods;
- Controlled Current Methods;
- Potentiometric Endpoint Detection;
- 11. Amperometric Methods (Anodic Stripping Analysis)
- 12. Chemically modified electrodes (CME) Various kinds of CME preparation routes; Overview of processes at modified electrodes

### **Teaching method**

- Demonstration
- Lecture

### Assessment

• Mid exam	30%
Individual Assignment	.20%
• Final Exam	50%
• Total	100%

## References

1. Wang, J. Analytical Electrochemistry, 2nd Ed., Wiley - VCH, 2000.

2. Bard, A., and Faulkner, L. Electrochemical Methods: Fundamentals and Applications, Wiley, New York, 2001.

3. Delahay, P. New Instrumental Methods in Electrochemistry, Wiley, New York, 1954.

4. Galus, Z. Fundamentals of Electrochemical Analysis, Ellis-Harwood, Chichester, 1976.

5 Gileadi, E., Kirowa-Eisner, E. and Penciner, J. Interfacial Electrochemistry – An Experimental Approach, Addison – Wesley, Reading, 1975.

Course Title: Separation Science

Course Code: Chem.522 CR.Hrs: 2 ECTS: 3

Status of the Course: Compulsory

**Course Description** An advanced study of the theory, instrumentation, and analytical applications of chemical separation methods. Mass transport processes, Thermodynamic and molecular basis of equilibrium separations, Chromatography and theory of retention, Kinetic processes in chromatography, Chromatography of planar surfaces, HPLC instrumentation: Adsorption, partition, ion-exchange, size-exclusion, affinity and chiral chromatography; Gas chromatography, supercritical fluid chromatography and "hyphenated methods

Course Objectives Upon the successful completion of this course, students will be able to:

- Define separation
- Explain the basic principles of various separation processes
- Explain the equilibrium processes in separations
- Apply different separation techniques for various matrices
- Understand the theoretical principles of the various chromatographic techniques

• Explain the various parameters affecting the components-separation in the complex mixtures and describe the various parameters that could be controlled in order to obtain effective separation

• Distinguish the type of chromatographic system that can be applied for a particular class of compound in a given matrices

• Interpret the peaks and relate them to the particular compound utilizing the peaks that could be obtained for standard samples under question

• Apply each type of the chromatographic system to associated problems in food, environmental, biological and other matrices

## **Course Contents**

11. History and Introduction to Separations

- 11.1. Introduction
- 1.2 instrumentation and analytical applications of chemical separation methods
- 1.3 Equilibrium Processes in Separations
- 1.4 Mass transport processes in Separation
- 1.5 Non chromatographic separations based on phase equilibria (Solvent extraction: Liquid-

liquid extraction), Distillation, precipitation, sublimation, crystallization)

- 2. Principles of Chromatographic Techniques
- 2.1 Introduction to the Theoretical Principles
- 2.2 The Chromatographic Processes
- 2.3 Types of Chromatographic Separation
- 2.4 Retention in Chromatography
- 2.5 The Distribution Coefficient
- 2.6 Band Broadening in Chromatographic Separation
- 2.7 Chromatographic Theories
- 2.7.1 Rate Theory
- 2.7.2 Plate Theory
- 2.8 Resolution
- 2.8.1 Factors Affecting Resolution
- 2.8.2 Peak Tailing and Fronting

- **General Considerations**
- 3.1 Basic Apparatus in Gas Chromatography
- 3.1.1 Carrier Gas Supplies
- 3.1.2 Sample Introduction Units
- 3.1.3 The Stationary Phase
- 3.1.4 Detection Systems in Gas Chromatography
- 3.2 Variables in Gas Chromatographic Separations
- 3.2.1 Effect of Column Length
- 3.2.2 Effect of Carrier Gas Velocity
- 3.2.3 Effect of the Stationary Phase
- 3.2.4 Effect of Temperature
- 3.2.5 Effect of Solute Retention Factor Change in Solute Elution Order
- 3.2.7 Separation Efficiency under Temperature Controlled Conditions
- 3.3 Selected Applications
- 3.3.1 Components Identification
- 3.3.2 Quantitative Analysis
- 3.3.3 Environmental Applications
- 3.3.4 Biological and Food Applications
- 3.4 Gas-Solid Chromatography
- 3.5 Calibration techniques
- 3.5.1 External standard methods
- 3.5.2 Internal standard methods
- 14. Liquid Chromatography
- 4.1 General Considerations
- 4.1.1 Liquid Chromatographic Separation Modes
- 4.1.2 Retention
- 4.1.2.1 Retention Factor k and Column Dead-Time
- 4.1.2.2 Role of Separation Conditions and Sample Composition
- 4.1.3 Peak Width And The Column Plate Number N
- 4.1.4 Resolution And Method Development
- 4.1.4.1 Optimizing the Retention Factor k

- 4.1.4.2 Optimizing Selectivity  $\alpha$
- 4.1.4.3 Optimizing the Column Plate Number N
- 4.1.5 Sample Size Effects
- 4.1.5.1 Volume Overload: Effect of Sample Volume on Separation
- 4.1.5.2 Mass Overload: Effect of Sample Weight on Separation
- 4.1.5.3 Avoiding Problems due to Too Large a Sample,
- 4.1.5.4 Effect of Temperature in Liquid Chromatographic Separations
- 4.2 The Liquid Chromatographic Equipments
- 4.2.1 Mobile Phase Delivery Systems
- 4.2.2 Properties of Solvents Used in Liquid Chromatography
- 4.2.3 Columns and Stationary Phases
- 4.2.4 Detectors in Liquid Chromatographic Separation
- 4.3 Normal/Reversed-Phase Chromatographic Separations
- 4.4 Types of Liquid Chromatography
- 4.4.1 Adsorption Chromatography (Liquid-Solid Chromatography)
- 4.4.1.1 General remarks
- 4.4.1.2 Stationary phase
- 4.4.1.3 Choice of mobile phase
- 4.4.2 Partition Chromatography
- 4.4.2.1 Principle
- 4.4.2.2 Choice of solid support; bonded phase packing material
- 4.4.2.3 Normal phase chromatography
- 4.4.2.4 Reverse phase chromatography
- 4.4.3 Ion-Exchange Chromatography
- 4.4.3.1 Principle
- 4.4.3.2 Structure and properties of ion-exchange materials/resins
- 4.4.3.3 Elution techniques
- 4.4.4 Size-Exclusion Chromatography
- 4.4.4.1 Principle
- 4.4.4.2 Packing material
- 4.4.5 Affinity Chromatography

- 4.4.5.1 Principles
- 4.4.5.2 Column material
- 4.4.6 Chiral Chromatography
- 4.5 Solving Elution Problems in Liquid Chromatography
- 4.6 Analytical Liquid Chromatography
- 4.6.3 Qualitative Analysis
- 4.6.4 Trace Analysis
- 4.6.5 Quantitative analysis
- 4.6.6 Recovery
- 4.6.7 Peak Height and Peak Area Determination for Quantitative Analysis
- 4.7 Application
- 4.8 Liquid Chromatography versus Gas Chromatography
- 15. Ion Chromatography
- 5.1 Principle
- 5.2 Instrumentation
- 5.3 Application
- 6. Planar Chromatography
- **6.1** Theoretical Principles
- 6.2 Paper Chromatography
- 6.2.1 Apparatus and Developments
- 6.2.2 Choice of Solvent Systems, Advantages, Limitations and Applications
- 6.3 Thin Layer Chromatography (TLC)
- 6.3.1 Introduction and History of TLC
- 6.3.2 Methods of Development and Detection
- 6.3.3 Comparison with HPTLC and HPLC
- 17. Supercritical Fluid Chromatography
- 7.1 Supercritical fluid
- 7.2 Instrumentation
- Application Project work

Students will select any of the chromatographic techniques, optimize parameters and apply to real samples. The present their result to the class

### Assessment

• Mid exam	30%
• Individual assignment	20%
• Final Exam	50%
• Total	100%

### References

1. Seader, J.D., Henley, E.J., Separation Process Principles, 1st Edn (1998), John Wiley & Sons. Inc., New York.

2. Ahuja, S. Chromatography and Separation Science, Academic press, 4th edn (2003)

3. Karger, B.L., Snyder, L.R., Howarth, C. An Introduction to Separation Science, 2nd Edition (1973), John Wiley, New York.

4. Meloan, C.E. Chemical Separation, Wiley Interscience Publication

5. Smith F.J. Chromatographic Methods, 5th edn. Kluwer Academic Publisher

 Lloyd R. Snyder And Joseph J. Kirkland. Introduction To Modern Liquid Chromatography, (2010) 3rd Edn. A John Wiley & Sons, Inc.,

Course Title: Analytical Applications of Complex Equilibria and Modern Extraction

Techniques

Course Code: Chem.621 Cr. Hrs: 3 ECTS: 5

Status of the Course: Compulsory

**Pre-requisites:-**

**Course Description** Complex Formation Equilibria, Stability Constant of Complexes, Conditional Stability Constant of Complexes, Extraction Equilibria, Extraction of Chelates, Extraction of Ion Association Complexes, Sampling in Environmental and Biological Analysis, Sample Pre-treatment, Sample Clean up; Extraction Techniques, Solid-Phase Extraction, Solid Phase Micro Extraction, Supported Liquid Membrane Extraction, Ultrasonic Assisted Extraction, Microwave Assisted Extraction, and Supercritical Fluid Extraction, Accelerated solvent extraction Course Objectives Upon the successful completion of this course, students will be able to:

• Understand and explain the complex formation equilibria, extraction equilibria, protonation equilibria, dissociation equilibria

• understand the different types of complex formation: mononuclear complexation equilibria, polynuclear complexation equilibria, mixed ligand complexation equilibria

• understand the stepwise stability constants, overall stability constants, conditional stability constants, protonation constants,

• Determine average ligand numbers, mole-fractions, and related parameters

Apply the complex formation equilibria and extraction equilibria to the analysis of inorganic (metals) and organic components in the different types of samples (environmental, biological, air, water, soil)

- Define components and operation of common sample preparation methods.
- Assess the benefits and limitations of different extraction methods.
- Validate extraction efficiency.
- Determine an appropriate extraction and pre-concentration method for an analysis.

• Explain the different on-line, in-line, at-line and off-line sample preparation techniques and their basic principles

• Explain the basic steps of sample handling strategies

Explain the advantage and limitations of various modern sample preparation protocols

• Compare and contrast the advantage and limitations of modern sample preparation protocols over the traditional/conventional sample preparation techniques

# Course Content Part 1: Analytical Applications of Complex Equilibria

- 1. Introduction
- 2. Complexes and their properties
- 2.1 Elements of the chemistry of complexes
- 2.2 Equilibria
- 2.2.1 Complex formation equilibria
- 2.2.1.1 Equilibria of mononuclear complexes
- 2.2.1.2 Equilibria of polyunuclear complexes
- 2.2.2 Equilibria of acid-base reactions: protonation of ligands

- 2.3 Conditional equilibrium constants
- 2.3.1 Role of hydrogen ion concentration in complex formation
- 2.4 Factors affecting complex formation
- 2.4.1 The nature of the central ions
- 2.4.2 Properties of the ligands
- 3. Determination of equilibrium constants
- 3.1 Determination of protonation constants
- 3.2 Determination of stability constants
- 4. Analytical applications
- 5. Equilibria of organic reagents (ligands) in solutions
- 5.1 Partition equilibria of organic reagents (ligands) and their complexes
- 5.2 Extraction equilibria and ion-exchange equilibria
- 5.3 Extraction of metal chelates
- 5.4 Extraction constants
- 5.5 Distribution ratio
- 5.6 Selectivity of extraction of metal ions
- 5.7 Analytical applications of extraction equilibria
- Part II modern sample preparation techniques
- 6. Modern Sample preparation techniques in analytical chemistry
- 6.1 Introduction
- 6.2 Sample handling
- 6.2.1 Sampling
- 6.2.2 Sample preparation
- 6.2.2.1 Sample pre-treatment, pre-concentration and clean-up and extraction
- 6.2.2.2 Online, at-line, in-line and off-line cleanup protocols
- 6.3 Solid Phase Extraction
- 6.3.1 Basic SPE principles
- 6.3.2 SPE Mechanisms
- 6.3.3 SPE Sorbents
- 6.3.4 Application
- 6.4 Solid phase micro-extraction 6.4.1 Principle

- 6.4.2 Sorbents in SPE
- 6.4.3 Sorbent selection
- 6.4.4 Application
- 6.5 Molecularly imprinted polymer based extraction
- 6.5.1 Principle and synthesis of molecular imprinted polymers
- 6.5.2 Application techniques of molecularly imprinted polymer for extraction
- 6.5.3. Electrospum nano fibers
- 6.5.3.1 Preparation and characterization of electrospum nano fibers
- 6.5.3.2 Application of electrospum nanofibers for extraction
- 6.6 Membrane Based Sample Preparation Techniques
- 6.6.1 Membrane Classification
- 6.6.2 Porous membrane based extraction

6.6.2.1 Dialysis

- 6.6.2.2 electrodialysis
- 6.6.3 Non porous membrane based extraction
- 6.6.4 Liquid Membrane Extraction
- 6.6.4.1 Two-Phase Liquid Membrane Extractions
- 6.6.4.2 Three-Phase Liquid Membrane Extractions
- 6.6.4.3 Transport Mechanisms in Liquid Membranes
- 6.6.5 Supported Liquid Membrane Extraction

6.6.5.1 SLM Modules

- 6.6.5.2 Principles of SLM Extraction
- 6.6.5.3 Extraction Efficiency and Enrichment Factor
- 6.6.6. Hollow fiber based membrane extraction
- 6.7 Ultrasonic extraction
- 6.7.1 Principle
- 6.7.2 application
- 6.8 Microwave assisted extraction
- 6.8.1 Principle
- 6.8.2 Solvent selection
- 6.8.3 Application

- 6.9 Supercritical fluid extraction
- 6.9.1 Theoretical considerations
- 6.9.2 Instrumentation
- 6.9.3 Operational procedures
- 6.9.4 Advantages/Disadvantages
- 6.9.5 Application
- 6.10 Accelerated solvent extraction
- 6.10.1 Basic principle
- 6.10.2 Instrumentation
- 6.10.3 Modifiers
- 6.10.4 Advantages/Disadvantages
- 6.10.5 Application
- 6.11. Subcritical water extraction
- 6.11.1 Basic principle
- 6.11.2 Instrumentation
- 6.11.3 Advantages/Disadvantages
- 6.11.4. Application
- 7. Miniaturized liquid-liquid extraction
- 7.1 single drop micro-extraction
- 7.2 Dispersive liquid-liquid extraction
- 8. Sample preparation techniques for trace metals in environmental and biological samples
- 8.1 Dry ashing vs wet ashing techniques
- 8.2 Open vs closed system digestion
- 8.2.1 Digestion on a hot plate
- 8.2.2 Digestion an a reflux condenser
- 8.2.3 Microwave digestion Project on the application of selected sample preparation methods; students will be allowed to select one or more modern sample preparation techniques to extract biological or environmental samples and quantify using spectroscopic/chromatographic techniques.

## **Teaching method**

- Demonstration
- Lecture

## Assessment

• Total	100%
• Final Exam	50%
Individual Project	20%
• Mid exam	30%

# **References:**

1. J. Inczedy, Analytical Applications of Complex Equilibria, Ellis Horwood, Chichester, 1976.

2. Z. Holzbecher, L. Divis, M. Kral, L. Sucha, F. Vlacil, Handbook of Organic Reagents in Inorganic Analysis, Ellis Horwood, Chichester, 1976.

3. R.L. Pecsok, L.D. Shields, T. Cairns, and I.G. McWilliam, Modern Methods of Chemical Analysis, 2nd ed., John Wiley, New York, 1976.

4. G.W. Ewing, Instrumental Methods of Chemical Analysis, 5th ed., McGraw-Hill Book Co. Singapore, 1987.

5. Fray D. Christian, Analytical Chemistry, 6th ed., John Wiley and Sons: New York; 2004.

6. S. Mitra, Sample Preparation Techniques In Analytical Chemistry. 2003, John Wiley & Sons, Canada

7. D.A. Skoog, Fundamentals of analytical Chemistry, 7th edn

Course Title: Chemometrics and Quality Assurance in analytical Chemistry

Course Code: Chem. 522 Cr.Hrs 3 ECTS: 5

Status of the Course: Compulsory

**Pre-requisites:** 

# **Course Description**

Analytical measurements and chemometrics, Errors and error propagation, Statistics of Repeated Measurements; Selected Significance tests in Chemical Analysis; Quality Control: Sampling Applied to Quality Control; Method Validation; Making Analytical Measurements; Regression

Analysis: The Correlation Coefficients, Limits of Detection, Regression Lines

and Curve Fitting. Non-parametric and Robust Methods, Experimental Design, Optimization and Pattern Recognition, Collaborative Trials and Control Chart

Course Objectives Upon the successful completion of this course, students will be able to:

• Design experiment, extract chemical information from large number of data, statistical treatment of analytical data

- Do the analysis of variance (apply ANOVA )
- Determine correlation coefficients and regression coefficient
- Apply different statistical tests
- · Compare the means and variances of different sets of data
- Apply various multivariate data analysis techniques
- Explain various data validation techniques
- Understand why analytical measurements need to be made
- Understand the importance of producing reliable results
- Be able to define what is meant by 'quality
- Appreciate the need for quality assurance
- Understand the importance of setting up a quality management system
- Be able to define what is meant by quality assurance and quality control
- Be aware of some of the international quality standards

Understand the importance of sampling plans and appreciate the legal and statutory requirements

• Appreciate the importance of correct sample handling and storage

### **Course Content**

- 1. Introduction
- 1.1 What is Chemometrics?
- 1.2 Definition of terms
- 1.3 Describing a set of data
- 1.3.1 Describing small set of data
- 1.3.2 Describing a large set of data
- 1.3.3 The normal distribution

- 2. Errors in chemical analysis
- 2.1 Introduction
- 2.2 Type of errors
- 2.3 Error, bias and precision
- 2.4 Propagation of errors
- 2.5.Detection, estimation and correction of bias
- 3. Statistics of repeated measurements
- 3.1 Introduction
- 3.2 Distribution of repeated measurements
- 3.3 Confidence limit and confidence interval
- 3.4 Random sampling in normal populations
- 3.5 Applying the normal distribution
- 3.6 Significance tests
- 3.6.1 Introduction
- 3.6.2 Comparison of an experimental mean with a known value
- 3.6.3 Comparison of two experimental means
- 3.6.4 Paired t-test
- 3.6.5 One-sided and two-sided tests
- 3.6.6 F-test for the comparison of standard deviations
- 3.6.7 Outliers
- 3.7 Analysis of variance
- 3.8 Comparison of several means
- 3.9 The arithmetic of ANOVA calculations
- 3.10 The chi-squared test
- 3.11 Testing for normality of distribution
- 3.12 Conclusions from significance tests
- 4. Calibration methods: regression and correlation
- 4.1 Introduction
- 4.2 Calibration graphs in instrumental analysis
- 4.3 The product-moment correlation coefficient
- 4.4 The line of regression of y on x

- 4.5 Errors in the slope and intercept of the regression line
- 4.6 Calculation of a concentration and its random error
- 4.7 Limits of detection
- 4.8 The method of standard additions
- 4.9 Use of regression lines for comparing analytical methods
- 4.10 Curvilinear regression methods
- 5. Experimental design and optimization
- 5.1 Introduction
- 5.2 Randomization and blocking
- 5.3 Two-way ANOVA
- 5.4 Factorial design and other designs
- 6. Multivariate analysis
- 6.1 Introduction
- 6.2 Initial analysis
- 6.3 Principal component analysis
- 6.4 Cluster analysis
- 6.5 Discriminant analysis
- 6.6 Application of Multivariate analysis
- 7. General Principles of Quality Assurance and Quality Control
- 7.1 Introduction to Quality Assurance
- 7.2 Quality Management System, Quality Assurance (QA) and Quality Control (QC)
- 7.3 ISO17025:2005 Management and technical requirements.
- 8. Sampling applied to quality control
- 8.1 Sampling Defined
- 8.2 Types of Samples
- 9. Preparing for Analysis 9.1 Selecting the Method
- 9.2 Sources of Methods
- 9.3 Factors to Consider when Selecting a Method
- 9.4 Performance Criteria for Methods Used
- 9.5 Reasons for Incorrect Analytical Results
- 10. Method Validation parameters

## 10.1Selectivity

- 10.2 Precision (Reputability, intermediate reproducibility, reproducibility)
- 10.3Accuracy
- 10.4 Measurement Range, Limit of Detection (LOD) and Limit of Quantitation (LOQ)
- 10.5Robustness and Ruggedness Testing

## 10.6Uncertainty

- 11. Making Analytical Measurements
- 11.1Good Laboratory Practice
- 11.2Before Starting an Analysis
- 11.3 During the Analysis
- 11.4 After the Analysis
- 11.5Calibration and Verification of Measurement
- 11.6Achieving Metrological Traceability
- 11.7Reference Materials
- 11.8Chemical Standards
- 12. Data Treatment
- 12.1Essential statistics
- 12.2Control Charts
- 12.3Measurement Uncertainty
- 13. Benchmarking your laboratories
- 13.1 Proficiency testing schemes
- 13.2 Collaborative trials

# **Teaching method**

- Demonstration
- Lecture

## Assessment

• Mid exam	30%
• Individual report writing	.20%
• Final Exam	.50%

• Total......100%

# References

1. R.E. Bruns, I.S. Scarminio, B. de Barros Neto, Statistical design — Chemometrics, in data Handling in Science and Technology—Volume 25, Advisory Editors: S. Rutan and B. Walczak, Elsevier B.V., Amsterdam, 2006.

2. Paul Gemperline, Practical Guide to Chemometrics, CRC Press, Boca Raton, 2006.

3. R.G. Brereton, Applied Chemometrics for Scientists, John Wiley and Sons, Chichester, 2007

4. R. Caulcutt and R. Boddy, Statics for Analytical Chemist, 1st ed., Chapman and Hall: London; 1983.

5. M.A. Sharaf, D.L. Illman, B.R. Kowalski, Chemometrics, John Wiley and Sons: New York;

1986. 6. J.N. Miller and J.C. Miller, Statistics and Chemometrics for Analytical Chemistry, 4th ed., Pearson Practice Hall: England; 2000.

6. Prichard, E and Barwick, V. Quality assessment in analytical chemistry. John Wiley & Sons, Ltd, UK, 2007

7. John, K. A primer on quality in the analytical laboratory. CRC Press, Boca Raton, Florida, 2000

Course Title: Special Topics in Analytical Chemistry

Course Code: Chem.621 Cr. Hrs: 2

Prerequisite

# Elective course I for Special Topics in Analytical Chemistry (elective course)

**Course Description** The course focuses on current research topics in analytical chemistry. Topics may be selected from the following: Surface analysis; Applied analysis (Environmental Chemistry; Food Chemistry and analysis; Forensic analysis); Non-Aqueous Solution Chemistry.

# **Course Content**

1. Surface Analysis

Basic principle, instrumentation and application of x-ray diffraction, scanning electron microscopy, transmission electron microscopy, scanning probe microscopy techniques), flow injection systems, chemical sensors and biosensors.

2. Applied analysis

2.1 Environmental Analysis

2.1.1 Water Analysis: sampling and preservation of water. Determination of pH, EC,TDS, DO, CO2, akalinity (carbonate, bicarbonate, hydroxide and total), salinity, chloride, fluoride, sulphate, H2S, calcium, magnesium, sodium, potassium, iron (total ferrous and ferric), ammonia, nitrite, nitrate, phosphorous (total inorganic and organic), BOD, COD, phenols, surfactants, pesticides, E-Coli and total bacteria.

2.1.2 Quality of water, standards of raw and treated water, objectives of waste water treatment. A brief idea of sedimentation, coagulation and flocculation, filtration, disinfection of water

2.1.3 Activated sludge process, trickling filters, sludge treatment and disposal. Softening of water, corrosion and its control.

2.1.4 Removal of toxic compounds, refractory organics, and dissolved inorganic substances. Reverse osmosis.

2.1.5 Air Analysis: atmospheric pollution, classification of air pollutants, sources of air pollution and methods of control, sampling of aerosols, sampling of gaseous pollutants, analysis of SOx, NOx, CO- O2, hydrocarbons, particulates, effects of air pollutants on animals, ozone layer, chlorofluorocarbons, acid rain, greenhouse effect.

2.1.6 Soil/Sediment analysis: a brief idea of chemistry of soil. Trace element analysis in soil - B,Cd, Cu, Fe, Mn, Mo, Zn, Pb. Pesticides and pollution, classification and degradation ofpesticides, methods of pesticides analysis.

2.1.7 Sampling of soil, aquatic sediments, pH, electrical conductivity, redox potential, alkalinity, inorganic and organic contents.

2.1.8 Waste Management: waste management approaches - waste reduction, recycling, disposal.

2.1.9 Management of hazardous wastes, household waste, municipal and industrial wastescollection, transportation and disposal options.

2.2 Forensic Analysis

2.2.1 Forensics-basic principles and significance, history and development.

2.2.2 Crime definition, crime scene, protection and recording of crime scene, physical clues, processing of crime scene.

2.2.3 Finger prints: classification, conventional methods of development of fingerprintsfluorescent and chemical methods.

2.2.4 Application of laser and other radiations to development of latent finger print.

2.2.5 Foot prints, tyre marks, bite marks and lip prints

2.2.6 Forensic Ballistics-fire arms, classification and characteristics, analysis of gunshot residues, mechanism of GSR, instrumental methods of GSR analysis.

2.2.7 Explosives: introduction, types, preliminary screening at crime scene, presumptive test (color and spot test), micro chemical methods of analysis

2.2.8 Fire Extinguishers and its chemistry, analysis of Arson exhibits by instrumental methods, management of flammable and combustible materials

2.2.9 Counterfeit coins-AAS analysis, purity of Gold-analysis by XRF / EDXRF

2.2.10 Forensic Toxicology: classification of poisons, estimation of poisons and drugs with

chromatographic, neutron activation analysis and spectrophotometric methods

2.3 Food Chemistry and Food Analysis

2.3.1 Food chemistry: definition and importance.

2.3.2 Water in food, water activity and shelf life of food.

2.3.3 Carbohydrates-chemical reactions, functional properties of sugars and polysaccharides in foods.

2.3.4 Lipids: classification and use of lipids in foods, physical and chemical properties, effects of processing on functional properties and nutritive value.

2.3.5 Protein and amino acids-physical and chemical properties, distribution, amount and functions of proteins in foods, functional properties, effect of processing-loss of vitamins and minerals due to processing.

2.3.6 Pigments in food, food flavours, browning reaction in foods.

2.3.7 Polyphenols distribution and importance in food.

2.3.8 Enzymes in foods and food industry, bio-deterioration of foods, food contaminants, additives and toxicants.

2.3.9 Principles of food processing: scope and importance of food processing. Principles and methods of food preservation-freezing, heating, dehydration, canning, addition of additives, fermentation, irradiation, extrusion cooking, hydrostatic pressure cooking, dielectric heating, microwave processing, aseptic processing, hurdle technology, membrane technology.

2.3.10 Storage of food-modified atmosphere packaging, refrigeration, freezing and drying of food, minimal processing, radiation processing.

2.3.11 Advanced techniques of food analysis: role of analysis and various methods of sampling and analysis of results.

2.3.12 Principles and application of flame photometry, atomic absorption, X-ray analysis, electrophoresis, mass spectroscopy, NMR, chromatography, refractometry, measurements, enzymatic methods, DSC, SEM, immunoassays, ESR. Analysis methods for total polyphenols, flavonoids, tannins and antioxidant activity assay.

# **Teaching method**

- Demonstration
- Lecture

# Assessment

• Individual presentation and term paper20%

# References

- 1. Jelen, P. Introduction to Food Processing, Prentice Hall, 1995.
- 2. Bailey R.A. Chemistry of the Environment, Academic Press, San Diego, 2000.
- 3. Baird C. Environmental Chemistry (2nd edition), WH Freeman and Co, 1999.
- 4. Bunce N. Environmental Chemistry, Wuerz Publishing Ltd., Winnipeg, Canada, 1991.
- 5. Cheremisinoff, N.P. Biotechnology for Waste and Wastewater Treatment, William Andrew, 1996.

6. Spiro, T.G. Purvis-Roberts, K., Stigliani, W.M. Chemistry of the Environment, University Science Books, 2011.

- 7. Wright, H. A Hand book of Soil Analysis, Logos Press, 1994.
- 8. Birch, G.G., Spencer, M., Cameron, A.G. Food Science, 3rd Edn., Pergamon Press, 1986.
- 9. Jelen, P.Introduction to Food Processing, Prentice Hall, 1995.
- 10. Fellows, P. Food Processing Technology: Principles and Practice, CRC Press, 2000.
- 11. Johari, M. Identification of Firearms, Ammunition and Firearm Injuries, BPR&D, 1980.

12. Nanda, B.B., Tewari, R.K. Forensic Science in India: A Vision for the Twentyfirst Century, Select Pub., 2001.

# Elective Course II for Special Topics in Analytical Chemistry Non-Aqueous Solution

**Chemistry Course Description** Introduction, Solvent-Solute Interactions (Intermolecular Forces, The Nature of Solvation), General Features and Characteristics of Non-Aqueous Solvents (Classification of Solvents, Physicochemical Properties of Typical Solvents), Correlation Properties in Different Solvents (Thermodynamic Transfer Functions, Transfer Functions for single Ions and Their Applications, Advanced Treatment of Acid-Base Chemistry

Objectives of the Course Upon completion of this module the students will be able to:

• Understand and explain the differences in the behavior of substances and their chemical reactions in the aqueous and non-aqueous solvents

• Able to understand the differences in the strength of acids and base and pH, standard electrode potentials, solubility, equilibrium constants, rate constants, in different solvents

• Able to correlate the strength of acids and base, the pH, standard electrode potentials, solubility, equilibrium constants, rate constants, in different solvents

• Apply the theoretical knowledge in quantitative and qualitative analytical applications of acidbase titrations, standard electrode potentials, etc.

# **Course Content**

- 1. Introduction
- 2. Solvent-Solute Interactions
- 2.1. Intermolecular forces
- 2.1.1. Ion-Ion Interactions
- 2.1.2. Ion-Dipole Interactions
- 2.1.3. Ion-Quadrupole Interactions
- 2.1.4. Ion-Induced Dipole Interactions
- 2.1.5. Dipole-Dipole Interactions
- 2.1.6. Dipole-Induced Dipole Interactions
- 2.1.7. Dispersion or London Interactions

- 2.1.8. Hydrogen Bonding
- 2.1.9. Specific Chemical Interactions
- 2.2. The Nature of Solvation
- 2.2.1. The Process of Solution
- 2.2.2. Solvation of Uncharged Molecules
- 2.2.3. Solvation of Ions
- 3. General Features and Characteristics of Non-aqueous Solvents
- 3.1. Classification of Solvents
- 3.2.1. Organic and Amphiprotic Inorganic Solvents
- 3.2.2. The Role of Hydrogen Bonding
- 3.2.3. Other Classification Schemes for organic Solvents
- 3.2.4. Inorganic Aprotic Solvents
- 3.2. Physico-chemical Properties of Typical Solvents
- 3.2.1. Water A Natural Amphiprotic Solvent
- 3.2.2. Acetic Acid A Protogenic Solvent
- 3.2.3. Liquid Ammonia A Protophilic Solvent
- 3.2.4. Acetonitrile A Dipolar Aprotic Solvent
- 3.2.5. Benzene An Inert Solvent
- 3.2.6. Liquid Sulfur Dioxide A Molecular Inorganic Solvent
- 3.2.7. Arsenic Trichloride An Amphoteric Inorganic Solvent
- 4. Correlation of Properties in Different Solvents
- 4.1. Thermodynamic Transfer Functions
- 4.1.1. Definitions and General Applications
- 4.1.2. Determinations of Thermodynamic Transfer Functions
- 4.1.3. Discussions of Representative Data
- 4.2. Transfer Functions for Single Ions and Their Applications
- 4.2.1. Estimation of Transfer Function for Single Ions

4.2.2. Interpretations of Transfer Functions for Single Ions obtained by the Tetraphenylborate Assumptions

- 4.2.3. Some Applications of the Transfer Activity Coefficients for Single Ions
- 5. Acid-Base Chemistry

- 5.1. Concepts of Acidity
- 5.1.1. Arrhenius Theory
- 5.1.2. Bronsted Concept
- 5.1.3. Lewis Concept
- 5.1.4. Usanovich Concept
- 5.2. Acidity Scales for Protonic Acids
- 5.2.1. Measurements and Interpretation of pH
- 5.2.2. Acidity Functions Based on Indicators
- 5.3. Acid-Base Titrations
- 5.3.1. Titration of Bases
- 5.3.2. Titration of Acids
- 5.3.3. Theoretical Bases for the Differentiation of the Strength of Acids and Bases in Dipolar

Aprotic Solvents

- 5.4. Quantitative Treatment of Acid-Base Equilibria
- 5.4.1. Equilibria in Acetic Acid
- 5.4.2. Equilibria in Acetonitrile

# **Teaching method**

- Demonstration
- Lecture

## **Mode of Assessment**

• Mid exam	.300%
• Individual presentation and term paper	20%
• Final exam	50%
• Total	.100%

## References

1. O. Popovych and R. P.T. Tomkins, Non-aqueous Solution Chemistry, John Wiley and Sons, Toronto, 1981.

2. T.C. Waddington, Non-Aqueous Solvents, Appleton-Century-Crofts, Educational Division, New York, 1969.

3. D.C. Harris, Quantitative Chemical Analysis, 4th ed., Freeman & Co., New York, 1995. 4.G.D. Christian, Analytical Chemistry, John Wiley and Sons, New York, 1995.

**Course Title:** Scientific Writing and Research Methodology **Course Code:** Chem. 552

#### Cr.Hrs: 2 ECTS: 3 Status of the Course: Compulsory

### **Pre-requisites:** -

**Course Description** Information searching, scientific writing and presentation skills, preparation of research proposals, laboratory techniques and safety in the laboratory, data analysis, and the use of computers in a chemical research will be covered.

### **Objectives of the Course**

The student gets an introduction to scientific research methods and will learn to make a report based on search in scientific databases, related to a work within his/her own field of research. The student will be familiar with the resources in the laboratory and will learn to obtain, evaluate and put together relevant information and learn to plan and document his/her scientific work in a constructive way. Students will be trained in oral and written presentation of their results.

**Course content** What is scientific research? Types of scientific research methods, Theories and background information about scientific theories and dialogs, Search for scientific publications in databases. The importance of written documentation in the scientific process, with emphasis on journals, report and the article. To write a scientific publication, style of writing according to form and content, correct way of writing and the use of references, Oral scientific presentation and popular scientific presentation, responsibility and ethics, Approach around scientific communication, publication bias and cheating in scientific research

Course Title: Seminar-I Course Code: Chem.591 Cr.Hrs: 1 ECTS: 2 Status of the Course: Compulsory Pre-requisites: -

### **Course Description**

The purpose of this course is to help students develop the necessary skills to communicate their knowledge to their colleagues and the public at large. It would entail organizing the content, oral delivery and proper write-up of a particular finding or research results. The skills required to do this will be discussed and practiced by writing a seminar paper and by defending in a seminar. The topics will likely be tilted toward organic Chemistry and its application to understanding synthetic phenomena.

Course Title: Thesis Course Code: Chem.698 Cr.Hrs: 6 ECTS: 10

Status of the Course: Compulsory

### Pre-requisites: -

## **Course Description**

Research project will be selected by students in topics which are of particular interest to them in consultation with their supervisors approved by the program. Students carry out experiments under the supervision of research teaching staff according to an original research theme. Students spend one year on experiments for research and obtain new knowledge and skills as they plan and carry out investigations and experiments. Projects can also be executed in collaboration with other concerned institutions. Their experiments will be summed up in a thesis and defended. Therefore, the course includes activities such as problem identification, literature survey, proposal writing and defense, laboratory work, thesis writing and final defense.

# 7. Responsible bodies to implement the curriculum

- Top managements of the University
- Post graduate director and coordinator of the University
- College of natural and computational science
- Department of chemistry and all staff members

### 8. References for the curriculum Design

- 1. Bahr Dar University, Curriculum for Masters of Science in Chemistry, March 2013.
- 2. Wollega University, current Master of Science curriculum, 2014.
- 3. Mekelle University Curriculum for Graduate Program (M.Sc.) in Chemistry
- 4. Gonder University, Master of Science Curriculum, 2009.
- 5. Ambo University, Currently functioning Master of Science curriculum, 2009.
- 6. Jimma University, currently functioning Master of Science Curriculum, 2009.
- 7. Research-Based & Course-Based M.Sc. Programs in Chemistry, Department of Chemistry, Addis Ababa University, October 2008.

8. Debre Markos University, Curriculum for the Degree of Masters of Science (M.Sc.) in Chemistry March. 2016.