DESCRIPTION OF COURSES FOR

M.PHIL & PHD



INSTITUTE OF CHEMICAL SCIENCES UNIVERSITY OF SWAT

RECOMMENDED BY 3RD BOARD OF STUDIES HELD ON MAY 24, 2023 AND APPROVED BY 2ND BOARD OF FACULTY OF CHEMICAL SCIENCES HELD ON AUGUST 08, 2023

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^{*}Courses developed by the faculty members, recommended in 3rd board of studies held on May 24, 2023 and approved by the 2nd board of faculty of chemical sciences held on August 08, 2023.

 $^{^{*1}}$ developed by Dr. Fazal Mabood

^{*2} developed by Dr. Muhammad Omar

 $^{^{*3}}$ developed by Dr. Ihsanullah

Introduction

The description of courses for MPhil and PhD was presented before the board of studies in its meeting scheduled on May 24, 2023 for recommendations and approval.

The board of studies includes following worthy members

1.	Prof. Dr. Fazal Mabood, Professor, Director ICS, UoS	Convener
2.	Dr. Ihsanullah, Assistant Professor, ICS, UoS	Member
3.	Dr. Muhammad Omer, Assistant Professor, ICS, UoS	Member
4.	Dr. Adnan, Assistant Professor, ICS, UoS	Member
5.	Dr. Mohammad Sohail, Assistant Professor, ICS, UoS	Member
6.	Dr. Ahmad Ali, Associate Professor, CPS&B, UoS	Member
7.	Dr. Azmat Ullah, Associate Professor, Deptt: of Chemistry, GPGJC, Swat	Member
8.	Dr. Nasir Ullah, Assistant Professor, Deptt: of Chemistry, GPGJC, Swat	Member
9.	Dr. Farman Ullah, Lecturer, Deptt: of Chemistry, GPGJC, Swat	Member
10.	Prof. Dr. Mumtaz Ali, Professor / Principal Govt. Degree College,	Expert
	Madyan, Swat.	
11.	Prof. Dr. Nasrullah Shah, Professor, Deptt: of Chemistry, AWKU, Mardan	Expert
12.	Dr. Anwar Hussain, Associate Professor / Chairman, Department of	Co-opt
	Economics and Developmental studies, Director ORIC-UoS	Member

Vision

To provide affordable quality education while equipping our graduates with knowledge and skills in their chosen stream of chemical sciences, provide opportunities for students to realize their full potential and thus shape them into future leaders in chemical sciences. We envision our institute to play a leading role in teaching and research and expect our graduates will serve the nation and humanity.

Mission

Our mission is the generation of quality human resources in the area of chemistry by producing highly skilled and well-trained graduates and researchers capable enough to address the future challenges both at regional and international levels.

Apart from teaching to develop the conceptual and problem-solving skills in our students, our mission is to cultivate an enthusiastic research culture by establishing laboratories equipped with sophisticated research facilities and establishing strong collaborations with other national and international institutions.

Objectives:

- To impart knowledge and training to students of BS, M.Phil and Ph.D levels in the field of Chemistry in various specializations to create a cadre of chemists who could perform adequately in the area.
- To educate students to be scientifically literate and provide them opportunities for professional growth through designing and executing chemical research projects.
 To establish research collaborations with relevant departments/institutes/research centers at national and international level.

Key to Course Coding

The course codes are composed of both letters and digits separated by hyphen. The letter CH denotes the chemistry course while digits have been started with 7 for MPhil level courses and 8 for PhD level courses.

For example,

CH- 701 means MPhil level course while

CH-801 means PhD level course.

THE FOLLOWING SCHEME OF STUDIES WAS APPROVED BY THE BOARD OF STUDIES FOR MPHIL (2-YEAR) PROGRAMME IN CHEMISTRY

Semes	ter-I			
S.No.	Course Title*	Course Code**	Cr. Hrs.	Marks
1	Course-I*	CH-**	3 (3-0)	100
2	Course-II*	CH-**	3 (3-0)	100
3	Course-III*	CH-**	3 (3-0)	100
4	Course-IV*	CH-**	3 (3-0)	100
Semes	ter-II		l	
S.No.	Course Title*	Course Code**	Cr. Hrs.	Marks
5	Course-V*	CH-**	3 (3-0)	100
6	Course-VI*	CH-**	3 (3-0)	100
7	Course-VII*	CH-**	3 (3-0)	100
8	Course-VIII*	CH-**	3 (3-0)	100
Semes	ter-III & IV		•	I
9	Research / Thesis /	CH-790	6 (0-6)	200
	Seminar			
		Total	30 (24-	1000
			6)	

^{*} The courses will be selected from the given list of courses (on next page) specified for M-Phil level depending upon the availability of expertise.

^{**} Each course has its own specific course code.

After exhaustive discussion, different courses from different fields of Chemistry were finalized for MPhil level as following:

MPhil-Chemistry level courses

Analytic	cal Chemistry		Inorganic Chemistry		
Course	Course Title	Credit	Course	Course Title	Credit
Code		Hours	Code		Hours
CH-701	Separation	3-0	CH-721	Medicinal Inorganic	3-0
	Techniques			Chemistry	
CH-702	Analysis and	3-0	CH-722	Inorganic Electronic	3-0
	Characterization			Spectroscopy	
	of Polymers			Specific Scopy	
CH-703	Atomic	3-0	CH-723	Kinetics and	3-0
	Spectroscopy			Mechanisms of	
	Бреси озсору			Inorganic Reactions	
CH-704	Chromatographic	3-0	CH-724	Physical Methods in	3-0
	Methods of			Inorganic Chemistry	
	Analysis			morganie enemetry	
CH-705	Composite	3-0	CH-725	Inorganic Material	3-0
	Materials			Chemistry	
CH-706	Design of	3-0	CH-726	Special Topics in	3-0
	Experiment			Inorganic Chemistry	
CH-707	Applications of	3-0			
	Computer and				
	Multivariate				
	Statistical Analysis in				
	Chemistry				
CH-708	Supramolecular	3-0			
	Polymer Chemistry				
Organic Chemistry			Physical Chemistry		
	Course Title	Credit	Course	Course Title	Credit
Code	•	Hours	Code		Hours
CH-741	8	3-0	CH-761	A.1 1 . C1	3-0
	Synthesis-			Advanced Chemical	
	Retrosynthetic			Kinetics	
	Approach				

CH-742	Advanced Stereochemistry	3-0	CH-762	Chemical and Statistical	3-0
CH-743	Nuclear Magnetic Resonance in	3-0	CH-763	Thermodynamics	3-0
	Organic Chemistry			Quantum Chemistry	
CH-744	Biosynthesis of	3-0	CH-764	Molecular	3-0
	Natural Products			Spectroscopy	
CH-745	Reactive	3-0	CH-765		3-0
	Intermediates in			Environmental	
	Organic			Chemistry	
	Chemistry				
CH-746	Advanced	3-0	CH-766		3-0
	Heterocyclic			Colloid Chemistry	
	Chemistry				
CH-747	Advanced Mass	3-0	CH-767	D-1 01	3-0
	Spectrometry			Polymer Chemistry	
CH-748	Special Topics in	3-0	CH-768	TT /	3-0
	Organic			Heterogeneous	
	Chemistry			Catalysis	
CH-749	Medicinal	3-0			
	Chemistry				

THE FOLLOWING SCHEME OF STUDIES WAS APPROVED BY THE BOARD OF STUDIES FOR PhD (3-YEAR) PROGRAMME IN CHEMISTRY

Semes	ter-I						
S.No.	Course Title*	Course Code**	Cr. Hrs.	Marks			
1	Course-I*	CH-**	3 (3-0)	100			
2	Course-II*	CH-**	3 (3-0)	100			
3	Course-III*	CH-**	3 (3-0)	100			
Semes	ter-II	1	I				
S.No.	Course Title*	Course Code**	Cr. Hrs.	Marks			
4	Course-IV*	CH-**	3 (3-0)	100			
5	Course-V*	CH-**	3 (3-0)	100			
6	Course-VI*	CH-**	3 (3-0)	100			
Semes	Semester-III & IV						
7	Research / Thesis /	CH-890	12 (0-	400			
	Seminar		12)				
		Total	30 (18-	1000			
			12				

^{*} The courses will be selected from the given list of courses (on next page) specified for PhD level depending upon the availability of expertise.

^{**} Each course has its own specific course code.

PhD-Chemistry level courses

Analytic	al Chemistry		Inorgan	ic Chemistry	
Course	Course Title	Credit	Course	Course Title	Credit
Code		Hours	Code		Hours
CH-801		3-0	CH-821	Advanced	3-0
	Nana Chamiatry			Nuclear and	
	Nano Chemistry			Radiation	
				Chemistry	
CH-802	Nuclear Methods of	3-0	CH-822	Organo-	3-0
	Analysis			transition Metal	
	Miarysis			Chemistry	
CH-803	Advanced	3-0	CH-823	Bio-Inorganic	3-0
	Chromatographic			Chemistry	
	Techniques			Circinistry	
CH-804	Molecular	3-0	CH-824	Catalysis	3-0
	Spectroscopy				
CH-805	Advanced Analytical	3-0			
	Instrumental				
	Techniques				
CH-806	Advanced Thermal	3-0			
	Analysis				
CH-807	Advanced	3-0			
	Chemometrics				
CH-808	Applications of	3-0			
	Polymer Nanofibers				
Organic	Chemistry		Physical	l Chemistry	
Course	Course Title	Credit	Course	Course Title	Credit
Code		Hours	Code		Hours
CH-841	Modern Name	3-0	CH-861	Physical	3-0
	Reactions in Organic			Chemistry of	
	Synthesis			High Polymers	
CH-842	Computational	3-0	CH-862	Advanced	3-0
	Chemistry/Molecular			Surface	
	Modeling			Chemistry	
CH-843	Protecting Groups in	3-0	CH-863	Advanced	3-0
	Organic Synthesis			Solution	
	J J			Chemistry	

CH-844	Physical Organic Chemistry	3-0	CH-864	Tribology	3-0
CH-845	Advances in	3-0	CH-865	Recent Advances	3-0
	Chromatographic			in Physical	
	Techniques			Chemistry	
CH-846	Chemistry	f 3-0	CH-866	Advanced	3-0
	Isoprenoids and	l		Statistical	
	Steroids			Mechanics	
CH-847	Chemistry o	3-0 f	CH-867	Applied	3-0
	Glycosides	-		Chemical	
	0.2) 0.02.400			Thermodynamics	
CH-848	Chemistry o	f 3-0	CH-868	Theoretical and	3-0
	Organometallic			Computational	
	Compounds			Chemistry	
CH-849	Organic	3-0	CH-869	Chemistry of	3-0
	Photochemistry			Advance	
	,			Materials	
CH-850		3-0	CH-870	Advanced	3-0
	Organic Polymer	•		Techniques in	
	Chemistry			Physical	
				Chemistry	
CH-851	Pericyclic Reactions	3-0			
CH-852	Cheminformatics	3-0			
CH-853	Advanced	3-0			
	Stereoselective				
011.054	Synthesis	2.0			
CH-854	Special Organic	3-0			
011.055	Materials	2.0			
CH-855	Multicomponent	3-0			
OH 056	Reactions				
CH-856		1 3-0			
	Catalyzed Organic	;			
	Synthesis				

M.PHIL COURSES

ANALYTICAL CHEMISTRY

Course Code: CH-701

Credit hours: 03

Course Title: Separation Techniques

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the separation techniques required during the organic and inorganic synthesis.

COURSE CONTENTS:

Chromatography: Classification, Classic and Kinetic Theory, Solvent Extraction and Solid Phase Extraction, Gas Chromatography: separation process, sample injection, detectors, sample preparation, method development. High Performance Liquid Chromatography: Chromatographic process, columns and stationary phase, injection and detectors, method development for reversed phase separation, gradient separations. Fast Protein Liquid (FPLC): Principle and work flow, Chromatography Cation/ Anion exchange chromatography, hydrophobic interaction Chromatography. Optimization of conditions and calibration of Instrumentation. Exchange Chromatography, Ion gel chromatography. CAPILLARY ELECTROPHORESIS: Basic principle, Zeta potential and the phenomenon of Electro-osmosis, General instrumentation and applications. CENTRIFUGATION: Principle of Centrifugation, Working with Normal and Ultracentrifuges. Use of Density Gradient Differential Centrifugation for Separation of Cellular Components.

- 1- Analytical Chemistry, R. Kellner, J-M. Mermet, M. Otto, H.M. Widmer
- 2- Quantitative Chemical Analysis, Daniel.C.Harris
- 3-Practical Biochemistry, Principles and Techniques Editors: Keith Wilson and John Walker 4th edition 1997, Cambridge University Press
- 4- Fundamental Laboratory Approaches for Biochemistry and Biotechnology, Alaxander J Ninfa & David P Ballou Fitzgerald Science Press Inc. 1998 Bthesda, Maryland
- 5- Methods in Molecular Biology Book series Vol. 59, Protein Purification Protocols David Sheelan Humana Press 2004

6- Separation Methods in Biochemistry CJOR Morris & P Morris 2nd edition 1976 Pitman Publishing.

Credit hours: 03

Course Title: Analysis and Characterization of Polymers

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the analysis and characterization of polymers. The course will enable the students to carry out analysis of newly synthesized polymers.

COURSE CONTENTS:

The polymerization processes and techniques, various types of polymers, molecular weight distribution and its determination, polymer additives (plasticizers, stabilizers and fillers). Chemical analysis, GPC and other chromatographic methods of analysis. Thermal analysis of various polymers: TGA, DSC, glass transition temperature. Spectroscopic analysis: UV, FTIR and NMR techniques, Mechanical, Microscopic and X-ray diffraction analyses. Synthetic and degradation reactions.

- 1. J.M.G. Cowie, Polymers: Chemistry and Physics of Modern Materials, International Textbook Co., London (1973).
- 2. F.W. Billmeyer, Textbook of Polymer Science, 3rd ed., John Wiley & Sons, New York (1994).
- 3. CE. Carraher, Seymour/Carraher's Polymer Chemistry, s" ed., Revised and Expanded, Marcel Dekker, New York (2000).
- 4. A. Ravve, Principles of Polymer Chemistry, 2nded., Plenum Publishers, New York (2000).
- 5. F.W. Rillmeyer. Jr., Textbook of Polymer Science, John Wiley & Sons, New York (1994).
- 6. J.R. Fried, Polymer Science and Technology, Prentice Hall/PTR (1995).
- 7. CE. Carraher, Introduction to Polymer Chemistry, CRC Taylor and Francis Group, New York (2007).
- 8. J.R. Fried, Polymer Science and Technology, Prentice Hall PTR (1995).

- 9. A. Rudin, The Elements of Polymer Science and Engineering, Academic Press (1999).
- 10. T.R. Crompton, Analysis of Polymers: An Introduction, Pergamon Press (1989).
- 11. CE.Carraher, Jr., Polymer Chemistry, An Introduction, 4th ed., Marcel Dekker, Inc. (1992).

Credit Hours: 03

Course Title: Atomic Spectroscopy

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the atomic spectroscopy required during the characterization and analysis of synthesized compounds.

COURSE CONTENTS:

Atomic absorption spectroscopy basic principles, Atomization basic Process, types of atomizers, Various factors affecting atomization process, analytical parameters, basic instrumentation: line sources, wavelength selectors and detectors, applications in analytical chemistry. Types of interferences associated with AAS. Principles of atomic fluorescence, instrumentation; Laser source, atomizers, and detectors, effect of temperature on fluorescence efficiency, analytical parameters and analytical applications. Principles of flame photometry, instrumentation, application of flame photometry and interferences. Plasma based emission spectroscopy, instrumentation, analytical parameters and applications.

- 1. D.L. Pavia, G.M. Lamp and G.S. Kriz, Introduction to Spectroscopy, 3rded .Thomson Learning, Inc., U.K. (2001).
- 2. Robert D. Braun, Introduction to Instrumental Analysis, McGraw Hill Book Co. New York.
- 3. Gary D. Christian, James E. O'Reilly, Instrumental Analysis, John Wiley and Sons.
- 4. Douglas A. Skoog, Stanley R. Crouch, Instrumental Analysis, Reinholt, New York.
- 5. F.W. Fifield and D. Kealy, Principles and Practice of Analytical Chemistry I.T.B, London.
- 6. Willard, Meritte and Dean, Instrumental Analysis, D. Van Nostrand, New York.
- 7. Bernhard Wetz, Atomic Absorption Spectroscopy, Verlay Chemie, New York.

Credit Hours: 03

Course Title: Chromatographic Methods of Analysis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the modern methods of chromatographic techniques that will be useful during the separation of mixture of compounds.

COURSE CONTENTS:

Introduction: Classification of chromatographic methods, theory of separations and retention characteristics, descriptions of chromatograms. Chromatographic parameters: The van-Deemter equation, column efficiency, band broadening and resolution. Quantitation techniques: Sample loading, loss of material on column, column packing, flow rates, detector response, batch separations, symmetrical and asymmetrical peaks. Types of liquid chromatography: Working methodology, instrumentation and applications of adsorption, partition, ion-exchange, gel permeation, affinity and high performance liquid chromatography, effect of temperature, particle size, column size, pressure and HETP. Detectors for liquid chromatography: High performance thin layer chromatography. Gas-Chromatography: Sample introduction, splitters, columns and detectors in GC, optimization of gas-chromatographic separations. Supercritical fluid Chromatography: Working principle, instrumentation and applications. Gel-electrophoresis: Theory and applications.

- 1. D. Harvey, Modern Analytical Chemistry, McGraw-Hill Companies Inc. (2000).
- 2. K.A. Rubinson and J.F. Rubinson, Contemporary Instrumental Analysis, Prentice-Hall, Inc., USA (2000).
- 3. A. Braithwaite and F.J. Smith, Chromatographic Methods, Chapman and Hall, New York (1985). Supplementary Books
- 4. J. Weiss, Ion Chromatography, 2nd ed., VCH Publishers Inc, New York (1995).
- 5. F. Rouessac and A. Rouessac, Chemical Analysis Modern Instrumental Methods and Techniques, John Wiley & Sons, Ltd., UK (2000).

- 6. G.D. Christian, Analytical Chemistry, 6th ed., John Wiley & Sons Ltd., Singapore (2003).
- 7. D.A. Skoog and J.J. Leary, Principles of Instrumental Analysis, 4th ed., Saunders College Publishing, USA (1992).
- 8. D.C. Harris, Quantitative Chemical Analysis, 3rd ed., W.H. Freeman Company, New York (1991).
- 9. R.D. Braun, Introduction to Instrumental Analysis, McGraw-Hill Book Company (1987).
- 10.R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, Analytical Chemistry, 2nd ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).

Credit Hours: 03

Course Title: Composite Materials

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the composite materials, their synthesis and characterization.

COURSE CONTENTS:

Materials, composite materials and their classification, matrices and reinforcements for composites. Reinforcements-matrix interface properties and processing of composites with metallic, ceramic and polymeric matrices. Mechanical, dynamic mechanical and thermal properties of composite materials. Toughening mechanisms and mechanical failure in polymeric composites. Spectroscopic and microscopic analyses.

- 1. D.D.L. Chung, Composite Materials: Functional Material of Modern Technologies, Springer-Verlag, London (2003).
- 2. F.L. Mathews and R.D. Rawlings, Composite Materials: Engineering and Science, Chapman and Hall, London (1994).
- 3. T.L. Vigo and B.J. Kinzig, Composite Applications: The role of Matrix, Fiber and Interface, VCH, New York (1992).
- 4. B.C. Hoskin and A.A. Baker, Composite Materials for Aircraft Structures, American Institute of Aeronautics and Astronautics, Inc. New York (1986).
- 5. M.M. Schwartz, Composite Materials: Processing, Fabrication and Applications, Prentice Hall, PTR, New Jersey (1997).
- 6. L. Nicolais and G. Carotenuto, Metal-Polymer, Nanocomposites, Wiley Interscience (2005).
- 7. T.S. Pinnavaia and G.W. Beall, Polymer-Clay Nanocomposites, John Wiley & Sons (2000).

Credit Hours:

03

Course Title:

Design of Experiment

COURSE LEARNING OBJECTIVES AND OUTCOMES:

This course enables students to fully appreciate the fundamental concepts and techniques of experimental design as well as the real-world value of design. It gives them a profound understanding of how design selection affects the information obtained in an experiment.

Students will acquire the importance of well-designed experiments and its application on chemical problem to extrapolate the rich amount of information hidden in each experimental problem, Application of Design Expert 11 a software package to design new experiment, Analyses and interpretation of the results obtained from complex multivariate data, Apply DoE to obtain maximum yield of the output variable with less number of input variables and also to minimize the error as well as the number of experiments and Train the students to apply obtained skills in their work place

COURSE CONTENTS:

Introduction to Designing Experiments

- About Designing Experiments
- Define Factor Constraints
- Add Interaction Terms
- Determine the Number of
- Check the Design
- Gather and Enter data
- Analyze the Results

Basic Principles of Design of Experiments

- Randomization
- Replication
- Blocking
- Confounding

Screening Design

- Two level Full Factorial Design with less than five factors
- Two level Fractional Factorial Design with less than five factors

Characterization Design

Factorial Designs

- When to Use? (Preliminary experiments)
- Full Factorial Design
- General Full Factorial Design
- Fractional Factorial Design
- Creating a Factorial Design
- Replication
- Blocking
- Analyzing a Factorial Design
- Interaction Plots
- Split Plot Designs
- Two level Full Factorial Design with less than five factors
- Two level Fractional Factorial Design with less than five factors
- Resolution III
- Resolution IV
- Resolution V

2^(k-p) Fractional Factorial Designs

- Basic Idea
- Generating the Design
- The Concept of Design Resolution
- Plackett-Burman (Hadamard Matrix) Designs for Screening
- Enhancing Design Resolution via Foldover
- Aliases of Interactions: Design Generators
- Blocking
- Replicating the Design
- Adding Center Points
- Analyzing the Results of a 2**(k-p) Experiment
- Graph Options

Response Surface Designs (Optimization)

- When to Use? (optimization)
- Central Composite Design
- Box Behnken Design
- Creating a Response Surface Design
- Analyzing a Response Surface Design
- Contour/Surface Plots

Split-Plot Designs

- What Is a Split Plot?
- When to Use? (Hard to change factors)
- Creating a Split Plot Design
- Analysis of a Split Plot
- Split-Split Plots
- Other Generalizations of Split Plots
- Repeated Measures
- Crossover Designs
- Further Reading and Extensions

Taguchi Methods: Robust Design Experiments

- Quality and Loss Functions
- Signal-to-Noise (S/N) Ratios
- Orthogonal Arrays
- Analyzing Designs
- Accumulation Analysis

Mixture designs and triangular surfaces

- Triangular Coordinates
- Triangular Surfaces and Contours
- The Canonical Form of Mixture Polynomials
- Common Models for Mixture Data
- Standard Designs for Mixture Experiments
- Lower Constraints
- Upper and Lower Constraints
- Analyzing Mixture Experiments
- Analysis of Variance
- Parameter Estimates
- Pseudo-Components
- Graph Options
- Designs for constrained surfaces and mixtures
- Overview
- Designs for Constrained Experimental Regions
- Linear Constraints
- The Piepel & Snee Algorithm
- Choosing Points for the Experiment
- Analyzing Designs for Constrained Surfaces and Mixtures

Practical & Tutorials

- One-Factor Categoric
- One-Factor Categoric (pt 2)
- Multilevel Categoric
- Multilevel Categoric (pt 2)
- Two-Level Factorial
- Fractional Factorial with Foldover
- Split-Plot Factorial
- Response Surface
- Response Surface (pt 2)
- Response Surface (pt 3)
- Optimal Design
- Split-Plot RSM
- Mixture Design
- Mixture Design (pt 2)
- Combined Mixture-Process
- RSM with Categoric Factors
- Historical Data
- Historical Data (pt 2)
- Combined Split-Plot Design

RECOMMENDED BOOKS / MATERIALS / REFERENCES:

- 1. https://www.statease.com/docs/v11/tutorials/index.html
- 2. https://www.statease.com/training/webinar.html
- 3. Statistics for Experimenters: Design, Innovation, and Discovery, 2nd Edition [Hardcover] George E. P. Box (Author) J. Stuart Hunter (Author), William G. Hunter (Author)
- 4. Design and Analysis of Experiments [Hardcover] Douglas C. Montgomery (Author)
- 5. Design of Experiments: An Introduction Based on Linear Models (Chapman & Hall/CRC Texts in Statistical Science) [Hardcover] Max Morris (Author)
- 6. Design and Analysis of Experiments (Springer Texts in Statistics) [Hardcover] Angela M. Dean (Author), Daniel Voss (Author)
- 7. Experiments: Planning, Analysis, and Optimization (Wiley Series in Probability and Statistics) [Hardcover] C. F. Jeff Wu (Author), Michael S. Hamada (Author)
- 8. Statistical Design and Analysis of Experiments, with Applications to Engineering and Science [Hardcover] Robert L. Mason (Author), Richard F. Gunst (Author), James L. Hess (Author) Statistical Design and Analysis of Experiments (Classics in Applied Mathematics No 22.) [Paperback] Peter W. M. John (Author)

Credit Hours:

Course Title:

Applications of Computer and Multivariate Statistical Analysis in

Chemistry

03

COURSE LEARNING OBJECTIVES AND OUTCOMES:

The course introduces advanced chemometric methods and their use on different kinds of multivariate

data of relevance for research and development. The students will acquire knowledge regarding survey

the common sampling techniques for inorganic and organic compounds and calculate necessary

sample size and number of samples in connection with sampling, explain the concept uncertainty;

identify and describe different contributions to the uncertainty and calculate the combined uncertainty,

apply statistical inference in the form of confidence intervals, t-test, F-test, one-way analysis of

variance and Chi-square test in chemical problems, perform simple linear regression with calculation

of confidence intervals for slope, intercept and predictions and calculate and interpret the correlation

coefficient, quantify and analyse results in writing and use statistical methods according to above to

assess and ensure the quality, describe the principles how multivariate data can be utilised for

classification and calibration, Apply of the techniques of regression and multifactor analysis of

variance.

COURSE CONTENTS:

Introduction to Data and Statistics

Introduction

• Univariate Statistics Review

• Variance and Sampling

• Linear Regression and Calibration

• Data, Digitization, and the Nyquist Theorem

• Detection Limit, S/N ratio, and Signal Filtering

Review of Linear Algebra

• Scalers, Vectors, and Matrices

• Matrix Notation and Matrix Operations

Orthogonality

Introduction to MatlabTM, SPSS, UOPUS, Unscramble

Page | 23

- Program Basics and Layout
- Matrix Operations
- The Diary Command and Examples

Multivariate Methods

- Introduction to Various Multivariate Methods
- The Six Habits of a Chemometrician
- Principle Component Analysis (PCA)
- Data Pretreatment: Mean Centering and Normalization
- PCA in MatlabTM

Multivariate Methods, Part II

- Classical Least Squares (CLS)
- CLS in MatlabTM
- Inverse Least Squares (ILS)
- ILS in MatlabTM

Multivariate Methods, Part III

- Multiple Linear Regression (MLR)
- Principle Component Regression (PCR)
- Partial Least Squares (PLS)
- Examples in using different software
- Summary of Multivariate Methods

Pattern Recognition

- Supervised *versus* Unsupervised Pattern Recognition
- K Nearest Neighbors (KNN)
- Soft Independent Modeling for Chemical Analysis (SIMCA)
- Summary of Pattern Recognition

Practical & Tutorials

Obtaining multivariate data by using analytical instruments like spectrophotometer, Spectroflourometer, chromatograph etc and then apply chemometrics for getting regression curve using softwares like Unscrambler, MATLAB, OPUS, SPSS etc

- 1. Total Synchronous fluorescence method for detection & quantification of extra virgin olive oil adulteration using Chemometrics,
- 2. Detection & quantification of extra virgin olive oil adulteration using Near Infra-red Spectroscopy and PLSDA Chemometric techniques

- 3. Determination of Methanol by using MIR spectroscopy combined with chemometrics
- 4. Determination of sugar contents in food sample using NIR combined with chempmetrics

RECOMMENDED BOOKS / MATERIALS / REFERENCES:

- Introduction to Multivariate Statistical Analysis in Chemometrics, Kurt Varmuza, Peter Filzmoser, CRC Press, 2009.
- 2. Multivariate Statistics, Hardle, Springer Science+Business Media, LLC, 2007.
- 3. Multivariate Data Analysis, Josep FH JR, 7th ed., Elsevier Inc, 2010.
- 4. Applied Multivariate Statistical Analysis, Richard A. Johnson, Dean W. Wichern, 6th ed., Pearson Education Inc, 2007.
- 5. Theory of Multivariate Statistics, Martin Bilodeau, David Brenner, Springer Media New York, 1999.
- 6. Linear Model Theory Univariate, Multivariate, and Mixed Models Wiley Series in Probability and Statistics, Keith E. Muller, Paul W. Stewart, A JOHN WILEY & SONS, INC., PUBLICATION, 2006.
- 7. Multivariate Data Analysis, Hair J.F., Black W.C., Babin B.J., Anderson R.E. 2010.
- 8. Applied Multivariate Data Analysis- Regression and Experimental Design, J. D. Jobson, Springer Science+Business Media New York, 1991.
- 9. Measurement and Multivariate Analysis, John C. Gower, Springer, 2002.
- 10. Regression Linear models in statistics, Bingham N., Fry J., Springer-Verlag London Limited, 2010.

Credit Hours: 03

Course Title: Supramolecular Polymer Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

This course provides about the deep insight of Supramolecular Polymer Chemistry. The students will learn

about the formation, bonding, different structures and also about the antibody and DNA catenanes.

COURSE CONTENTS:

Introduction

Formation of Supramolecular Polymers, Multiple hydrogen-bonded supramolecular polymers, Introduction,

General Concepts of Hydrogen-Bonding Motifs, Hydrogen-Bonded Main-Chain, Supramolecular Polymers,

From Supramolecular Polymers to Supramolecular Materials

Cyclodextrin-based supramolecular polymers

Introduction, Supramolecular Polymers in the Solid State, Formation of Homo-Intramolecular and

Intermolecular Complexes by CDs-Guest Conjugates, Formation of Intermolecular Complexes by CD and

Guest Dimers, Artificial Molecular Muscle Based on c2-Daisy Chain

Supra-macromolecular chemistry: toward design of new organic materials from supramolecular

standpoints

Introduction, Small Molecules, Macromolecules, and Supramolecules: Design of their Composite Materials

Polymerization with ditopic cavitand monomers

Introduction, Cavitands, Self-Assembly of Ditopic Cavitand Monomers, Supramolecular Polymers with Unique

Structures

Polymers containing covalently bonded and supramolecularly attached cyclodextrins as side groups

Polymers with Covalently Bonded Cyclodextrins as Side Groups, Side Chain Polyrotaxanes and

Polypseudorotaxanes

Antibody dendrimers and dna catenanes

Molecular Recognition in Biological Systems, Antibody Supramolecules, DNA Supramolecules

RECOMMENDED BOOKS:

Page | 26

- 1. Supramolecular Polymer Chemistry" by Alberto Ciferri and Jean-Marie Lehn. ISBN: 978-3527320950
- 2. Supramolecular Chemistry: Concepts and Perspectives" by Jean-Marie Lehn. ISBN: 978-3527292318
- 3. Supramolecular Chemistry: From Molecules to Nanomaterials" by Philip A. Gale and Jonathan W. Steed. ISBN: 978-1118483989
- 4. Supramolecular Polymer Networks and Gels" edited by Helmut Ritter and Eduard Brynda. ISBN: 978-3540890304
- 5. Supramolecular Polymer Chemistry: Scope and Perspectives" edited by Alberto Ciferri. ISBN: 978-1439837389
- 6. Supramolecular Polymer Networks: Synthesis, Properties, and Applications" edited by Roman Boulatov. ISBN: 978-3527330249
- 7. Supramolecular Polymers" edited by Alberto Ciferri. ISBN: 978-0849391775
- 8. Supramolecular Polymer Chemistry: Self-Assembled and Covalently Linked Systems" edited by Alexei R. Khokhlov and Sergei N. Chvalun. ISBN: 978-3527323920

INORGANIC CHEMISTRY

Course Code: CH-721

Credit Hours: 03

Course Title: Medicinal Inorganic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of medicinal inorganic compounds used during the treatment of different diseases. The course will enable the students to design synthesis of new drugs.

COURSE CONTENTS:

Introduction: General introduction to medicinal inorganic chemistry. Radiotherapy: Emitter therapy and radiopharmaceuticals. Metal complexes as pharmaceuticals: Anticancer drugs in chemotherapy, arthritis treatment, insulin mimics. Chelate Compounds: Chelation therapy for metal-related diseases and toxicity, nanotechnology in biomedicine.

- 1. S.J. Lippard and J.M. Berg, Principle of Bioinorganic Chemistry, University Science Books (1994).
- 2. R.W. Hay, Bioinorganic Chemistry, Ellis, Harwood, London (1991).
- 3. K.S. Coleman, Annu. Rep. Prog. Chem., Sect. A, 103, 392-406 (2007) (Review).
- 4. P.C. McGown, ibid, 101, 631-648 (2005) (Review).
- 5. D.S. Urch and M.J. Welch, ibid, 101, 585-606 (2005) (Review).

Credit Hours:

03

Course Title: Inorganic Electronic Spectroscopy

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the electronic spectroscopy.

The course will enable the students to carry out analysis of different inorganic complexes.

COURSE CONTENTS:

Term symbols, Russel Saunders, coupling scheme, development of correlation and Tanabe-

Sugano diagrams, crystal field diagrams. Energy level calculations; selection rules, band

intensities and band assignments. Interpretation of crystal field and charge transfer

spectra. Spectra of low symmetry complexes. Application of group theory to vibrational

spectra of simple and coordination compounds.

RECOMMENDED BOOKS:

1. A.B.P. Lever, Introduction to Electronic Spectroscopy, Elsevier, Amsterdam (1968).

2. J.P. Facler, Symmetry in Coordination Chemistry, Academic Press, New York (1971).

3. Alan and Vincent, Molecular Symmetry and Group Theory, John Wiley, London (1977).

4. F.A. Cotton, Chemical Applications of Group Theory, 3rd ed., John Wiley, New York

(1990).

5. J. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Addison-

Wesley, Reading/Singapore (1993).

Credit Hours: 03

Course Title: Kinetics and Mechanisms of Inorganic Reactions

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the inorganic reactions regarding their mechanisms and kinetics. The course will enrich the students for designing the synthesis of inorganic compounds.

COURSE CONTENTS:

Principles of kinetics. Steady state approximation. Determination of rate law. Inert and labile complexes. Substitution reactions of octahedral, square planer and tetrahedral complexes. Oxidation-reduction reactions of metal ions. Organo-transition metal compounds. Free radical reactions.

- 1. D. Benson, Mechanisms of Inorganic Reaction in Solution: An Introduction, McGraw-Hill, London (1968).
- 2. F. Basolo and R.G. Pearson, Mechanisms of Inorganic Reactions: A Study of Metal Complexes in Solutions, 2nd ed., John Wiley, New York (1967).
- 3. D. Katakis and G. Gordon, Mechanisms of Inorganic Reactions, Wiley- Interscience, New York (1987).
- 4. S.R. Logan, Fundamentals of Chemical Kinetics, Longman, London (1996).
- 5. J.O. Edwards, Inorganic Reaction Mechanism: An Introduction, W.A. Benjamin, New York (1965).
- 6. R.C. Henderson, The Mechanisms of Reactions of Transition Metals, 5th ed. Oxford University Press (1993).

Credit Hours: 03

Course Title: Physical Methods in Inorganic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the different physical aspects of inorganic compounds. The course will enrich the students to carry out synthesis of targeted molecules.

COURSE CONTENTS:

Infrared and Raman spectroscopy and their applications. Group theory and vibrational analysis. Application of ORD, CD, NMR, ESR and Mass Spectrometry to inorganic systems.

- 1. J.B. Lambert and E.P. Mazzola, Nuclear Magnetic Resonance Spectroscopy, Prentice Hall, New Jersey, (2003).
- 2. D.L. Pavia, G.M. Lamp and G.S. Kriz, Introduction to Spectroscopy, 3rd ed., Thomson Learning, Inc., U.K. (2001).
- 3. R. Davis, M. Frearson, Mass Spectrometry, Analytical Chemistry by Open Learning, John Wiley and Sons, New York (1987).
- 4. C.G. Herbert, R.A.W. Johnstone, Mass Spectrometry, Basics, CRC Press London (2002).
- 5. M. Yonus, Organic Spectroscopy, AHP International (Pvt.) Ltd. Lahore, (1998).

03

Credit Hours:

Course Title: Inorganic Material Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about different inorganic materials. The course will enrich the students with the chemistry of materials and design synthesis of new inorganic materials.

COURSE CONTENTS:

Introduction to inorganic materials, Application and interpretation of powder X-ray diffraction data of materials, The synthesis of inorganic materials – Solid state reactions, Precursor, solution and sol-gel methods, Solid-gas reactions, Hydrothermal method, CVD, Aerosol process, Low temperature method, Transition metal oxides, Electronic, magnetic and optical properties of inorganic materials, Nonstoichiometric compounds, Zeolites, intercalation in layer materials and solid electrolytes, Some recent developments in inorganic material chemistry.

- 1. M.T. Weller, Inorganic Material Chemistry, Oxford University Press, Inc., New York (1994).
- 2. L. Smart and E. Moore, Solid State Chemistry, 2nd ed., Chapman & Hall (2004).
- 3. A.R. West, Basic Solid State Chemistry, 2nd ed., John Wiley & Sons, Ltd. (2000).

Credit Hours: 03

Course Title: Special Topics in Inorganic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about recent research topics that are carried out in the field of inorganic chemistry.

COURSE CONTENTS:

Topics under recent investigation and of current interest (the choice will depend upon the interests of the teacher giving this course).

ORGANIC CHEMISTRY

Course Code: CH-741

Credit Hours: 03

Course Title: Organic Synthesis-Retrosynthetic Approach

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding to design protocols for synthesis of small to medium sized organic compounds and be able to carry out retrosynthetic analysis and propose alternative reactions to synthesize a compound.

COURSE CONTENTS:

Introduction: Basic definitions of retrosynthesis and disconnection approach. **Synthesis of aromatic compounds:** One and two group C-X disconnections. **Synthons:** Definitions and different types of donor and acceptor synthons, concept of "Umpolung". **C-C disconnections of difunctionalised compounds:** Dicarbonyl compounds such as 1,2; 1,3; 1,4; 1,5 and 1,6 diO compounds. **Synthesis of ring compounds:** Three, four, five six, seven and eight membered carbocycles and heterocycles. **Devising synthetic schemes:** Joint application of the concepts to unknown molecules and some natural products.

RECOMMENDED BOOKS:

1. S. Warren, Organic Synthesis: the Disconnection Approach, John Wiley & Sons Ltd. (1992).

2. J. Clayden, N. Greeves. S. Warren and P. Worthers, *Organic Chemistry*, Oxford University Press (2001).

3. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Blackie Academic and Professional, London, 1993.

SUPPLEMENTARY BOOKS:

1. W. Carruthers, *Modern Method of Organic Synthesis*, Cambridge University Press (1971).

- 2. S. Warren, Designing Organic Syntheses, J. Wiley & Sons, Chichester (1982).
- 3. T.W. Greene and P.G.M. Wuts, *Protective Group in Organic Synthesis*, John Wiley & Sons, Inc (1999).
- 4. J. Fuhrhop and G. Penzlin, *Organic Synthesis*, 2nd Edition, VCH, Weinheim, Germany (1994).

03

Credit Hours:

Course Title: Advanced Stereochemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about structures and reactions of organic compounds in 3-Dimensions that will be helpful in the organic synthesis and characterization of compounds.

COURSE CONTENTS:

Configuration and conformation of cyclic molecules: Stereochemistry and conformational analysis of cyclohexane systems, six-membered sp2-hybridized cyclic systems, six-membered saturated heterocycles. Stereochemistry and conformational effects in ring systems: Small, common and medium bicyclic and polycyclic fused rings; bridged rings and stereochemical restrictions. Chiroptical properties: Optical rotatory dispersion (ORD) and circular dichroism (CD).

RECOMMENDED BOOKS:

- 1. E.L. Eliel, S.H. Wilen and M.P. Doyle, *Basic Organic Stereochemistry*, Wiley Interscience, New York (2003).
- 2. D. Nasipuri, *Stereochemistry of Organic Compounds-Principles and Applications*, New Age international Publishers (P) Limited, New Delhi, India (1991).
- 3. P.S. Kalsi, Stereochemistry and Mechanism Through Solved Problems, New Age International Publishers, New Delhi, India (2001).

SUPPLEMENTARY BOOKS:

- 1. J. Eames (Queen Mary and Westfield College, University of London) and J.M. Peach, *Stereochemistry at a Glance*, Blackwell Publishing (2003).
- 2. D.G. Morris, *Stereochemistry*, Royal Society of Chemistry, U.K. (2001). 3. R. Gabba, *Stereochemistry*, Campus Books International, New Delhi, India (2002).

Credit Hours:

03

Course Title: Nuclear Magnetic Resonance in Organic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the important characterization technique and be able to elucidate the structures of newly synthesized / novel organic

compounds.

COURSE CONTENTS:

Spin couplings: Spin coupling in different spin systems. Double resonance experiments: Spin decoupling in 1H- and 13C-NMR spectroscopy, suppression of solvent signal, 1H BB decoupling, gated decoupling, 1H off-resonance decoupling. 1D NMR experiments with complex pulse sequence: The *J*-modulated spin echo, SPI, INEPT and DEPT experiments. 2D NMR Spectroscopy: Introduction, theory and presentation of 2D spectrum. 2D *J*-resolved NMR spectroscopy: Homo- and hetero-nuclear 2D *J*resolved NMR spectroscopy. 2D shift-correlated NMR spectroscopy: H,H-COSY, H,C-COSY, NOESY, ROESY, HMBC,

HMQC and TOCSY experiments. **Applications:** NMR use as a tool for structure elucidation

and stereochemical assignments.

RECOMMENDED BOOKS:

1. H. Friebolin, *Basic one-and two-dimensional NMR spectroscopy*, 4th ed., Wiley- VCH,

New York (2005).

2. D. Canet, Nuclear magnetic resonance: concepts and methods, John Wiley & Sons,

Chichester, England (1996).

3. Atta-ur-Rehman and M.I. Chaudhry, Solving problems with NMR spectroscopy,

Academic Press, California (1996).

4. R. M. Silverstein, F. X. Webster and D. J. Kiemle, Spectrometric identification of

organic compounds, John Wiley & sons Inc., USA (2005).

SUPPLEMENTARY BOOKS:

1. R.S. Macomber, NMR spectroscopy: basic principles and applications, Harcourt Brace

Jovanovich Publishers, San Diego (1988).

- 2. S. Berger and S. Braun, 200 and more NMR experiments, Wiley-VCH, Weinheim, Germany (2004).
- 3. Handbook of proton-nmr spectra and data, Asahi Research Center Co., Academic Press, New York (1985).
- 4. J.K.M. Sanders, et al., *Modern NMR spectroscopy: a guide for chemists*, The University Press, Oxford (1993).
- 5. Breitmaier and Eberhard, Structure elucidation by NMR in organic chemistry: a practical guide, John Wiley, West Sussex (2002).
- 6. Y.C. Ning, Spectral Identification of organic compounds with spectroscopic techniques, Wiley-VCH, Weinheim (2005).

Credit Hours: 03

Course Title: Biosynthesis of Natural Products

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the secondary metabolites and their biosynthesis that will be helpful to understand and carry out the total synthesis of natural products.

COURSE CONTENTS:

Introduction: Classification of natural products, primary and secondary metabolites, enzymes and coenzymes. **Biosynthesis:** Fatty acids, polyketides, isoprenoids, amino acids and alkaloids. **Metabolites from shikimic acid:** ArC1, ArC2 and ArC3 metabolites. **Mixed biosynthesis:** Metabolites derived from acetate and mevalonate, shikimate and mevalonate, acetate and shikimate, tryptophan and mevalonate.

RECOMMENDED BOOKS:

- 1. S.P. Stanforth, *Natural Product Chemistry at a Glance*, Oxford: Blackwell (2006).
- 2. J. Mann, Secondary Metabolism, Oxford Science Publications, (1987).
- 3. J.D. Bu'Lock, *The Biosynthesis of Natural Products*, McGraw-Hill, London (1965).

SUPPLEMENTARY BOOKS:

- 1. S. Ranganathan, Art in Biosynthesis, Academic Press, New York (1976).
- 2. R.H. Thomson (Ed.), *The Chemistry of Natural Products*, 2nd ed., Springer- Verlag New York, LLC (1993).
- 3. R.B. Herbert, *The Biosynthesis of Secondary Metabolites*, Springer-Verlag, New York, LLC (1989).
- 4. K. Nakanishi, T. Goto, S. Ioto, S. Natori, S. Nozone, et al., *Natural Products Chemistry*, Vol. 1, Academic Press Inc, New York (1974).

Credit Hours:

03

Course Title: Reactive Intermediates in Organic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the reactive intermediates that

will be helpful to understand the reaction mechanism of organic reactions and design the

synthesis of novel and new compounds.

COURSE CONTENTS:

Introduction: Reactive intermediates and transition states. Carbocations: Classical and

non-classical carbocations, reactions of non-classical carbocations with stereochemical

aspects, pericyclic reactions involving carbocations. Carbanions: Generation of carbanions,

kinetic and thermodynamic control, stability and reactions, carbanions stabilized by

heteroatoms, rearrangements. Free radicals, carbenes, nitrenes and arynes: Generation

and reactions, relative stability and stereochemical aspects of reactions.

RECOMMENDED BOOKS:

1. R. A. Moss, M. S. Platz and Maitland Jr. (Eds.), Reactive Intermediate Chemistry,

Jones. Wi (2004).

2. N. Issac, Reactive Intermediate in Organic Chemistry, John Wiley and Sons (1974).

3. M. Jones and R. A. Moss, *Reactive Intermediates*, John Wiley and Sons, New York

(1978).

SUPPLEMENTARY BOOK:

1. M.B. Smith and J. March, March's Advanced Organic Chemistry: Reactions,

Mechanisms, and Structure, John Wiley & Sons (2007).

03

Credit Hours:

Course Title:

Advanced Heterocyclic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of heterocyclic compounds that is important in the designing of synthesis of pharmacologically important new and novel compounds.

COURSE CONTENTS:

Oxygen, nitrogen and sulphur containing heterocycles: Synthesis, reactions, stereochemistry and spectroscopy. Heterocycles with more than one heteroatom: Synthesis, reactions and spectroscopy of five - seven membered heterocycles. Fused ring systems: Benzofused five - seven membered heterocycles.

RECOMMENDED BOOKS:

- 1. H. El-Syed, *Heterocyclic Chemistry*, Blackwell Publishing (2006).
- 2. J. Joule, Synthesis of Naturally Occurring Heterocycles from Carbohydrates, Blackwell Publishing (2006).
- 3. R.K. Bansel, *Heterocyclic Chemistry*, New Age International, New Delhi (1996).

SUPPLEMENTARY BOOKS:

- 1. R.H. Acheson, *An Introduction to Chemistry of Heterocycles Compounds*, 3rd ed., John Wiley, New York (1976).
- 2. J.M. Loudon, Organic Chemistry, Oxford University Press (2002).
- 3. F.A. Carey, R.J. Sandberg, *Advance Organic Chemistry*, Kulver Academic/ Plenum Publisher (2000).

Credit Hours: 03

Course Title: Advanced Mass Spectrometry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the important characterization technique that will be helpful in the elucidation of newly synthesized compounds.

COURSE CONTENTS:

Introduction: Aims and scope, theory and basic terminology. **Instrumentation:** Instrumental design, ionization techniques, types of analyzers and detectors. **Applications:** Modes of fragmentation of various organic compounds, interpretation of mass spectra of unknown organic compounds.

RECOMMENDED BOOKS:

- 1. C.G. Herbert and D.P. Schulz, *Mass Spectrometry Basics*, Taylor & Francis, New York (2003).
- 2. F.W. McLafferty, F. Turecek and J. Choi, *Interpretation of Mass Spectra*, University Science Books, California (1993).
- 3. E. De Hoffmann, J. Charette and V. Stroobant, Mass Spectrometry, Principles & Applications, John Willey & sons (1996).

SUPPLEMENTARY BOOKS:

- 1. J.H. Gross, Mass Spectrometry, Springer-Verlag New York (2004).
- 2. A.Frigerio, Essential Aspects of Mass Spectrometry, Spectrum Publications Inc. New York (1974).
- 3. H.E. Duckworth, R.C. Barber and V.S. Venkatasubramanian, *Mass Spectroscopy*, Cambridge University Press, London (1986).
- 4. R.E. Ardrey, Liquid Chromatography Mass Spectrometry: An Introduction, John Wiley & Sons (2003).

5. S.M. Nelms, *Inductively Coupled Plasma Mass Spectrometry Handbook*, Taylor & Francis, New York (2005).

Credit Hours: 03

Course Title: Special Topics in Organic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the different topics of recent research undertaken in the field of organic chemistry.

COURSE CONTENTS:

Topics under recent investigation and of current interest (the choice will depend upon the interests of the teacher giving this course).

Credit Hours:

Course Title: Medicinal Chemistry

03

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of medicines and different drugs. The knowledge will be helpful in the designing of new drugs.

COURSE CONTENTS:

Introduction: Historical perspectives of drug targets, pharmacokinetics and pharmacodynamics. Biological screening: Different types of bioassays, in vitro and in vivo testing of different compounds. Drug discovery: The lead compound, natural and synthetic sources of lead compounds. Drug synthesis: Combinatorial and solid phase synthesis of drug like compounds. Structure activity relationship: Calculation of molecular descriptors using different available software, Hansch analysis and use of Craig plots and Topliss scheme for the synthesis of lead analogs. Binding interactions: Different types of receptor-ligand interaction, functional group as binding groups and their bioisosters. Computer assisted drug designing: Generation of pharmacophore, receptor- and ligand-based drug designing.

RECOMMENDED BOOKS:

- 1. J.N. Delgado and W.A. Remens, *Textbook of Organic and Medicinal Chemistry*, 10th ed., Lippincolt William and Wilkins (1998), 11th ed. (2004).
- 2. C.L. Patrick, *Introduction to Medicinal Chemistry*, OUP (2001).
- 3. P.K. Larsen, *Drug Design and Development*, 2nd ed., Harward Academic Publishers (1996).

SUPPLEMENTARY BOOKS:

- 1. G. Thomas, Fundamentals of Medicinal Chemistry, John Wiley (2003).
- 2. Advanced Pharmaceutics, C.J CRC. Press (2004).
- 3. P. Sencer, Solid Phase Synthesis and Combinatorial Technologies, Wiley Intense (2000).
- 4. C.G. Wenments, *Medicinal Chemistry*, Academic Press (2004).

- 5. B. Yan, Analytical Methods in Combinatorial Chemistry, Technomic Publishers (2000).
- 6. R.B. Silverman, *The Organic Chemistry of Drug Design and Drug Action*, 2nd ed., Academic Press (2004).

PHYSICAL CHEMISTRY

Course Code: CH-761

Credit Hours: 03

Course Title: Advanced Chemical Kinetics

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding to fundamentals of kinetics, theories about kinetics of chemical reactions (elementary and complex) and experimental techniques required for kinetics. Students will also be able to utilize the knowledge in experimental work.

COURSE CONTENTS:

- 1 **Basic Kinetics Concepts:** Scope of chemical kinetics, Reaction Stoichiometry, rates of consumption and formation, Extent of Reaction, Rate of reaction, Empirical rate equation, Elementary, composite and Chain reactions
- Analysis of Kinetics Results: Differential Method, Method of integration, Isolation method, Half life method, Comparison of methods, Opposing reactions, Reaction in flow system, Correlation of physical properties with concentration, Conventional experimental techniques, Techniques for very fast reactions and influence of temperature on reaction rates
- 3 **Mechanism of Elementary Reactions:** Potential energy surfaces, Kinetic theory of collision, Conventional transition state theory and its application, Comparison of two theories, Thermo chemical formulation of transition state theory, Lindemann Christiansen hypothesis for uni-molecular reactions, Kinetics isotope effect.
- 4 **Reactions in solutions:** Solvent effect on reaction rate, Factors determining reaction rates in solution, Reaction between ion.
- 5 **Composite Reactions:** Parallel reactions, Consecutive reactions, steady state treatment, Reactions involving free radical mechanism,

- 1. P. L. Houston, Chemical Kinetics and Reaction Dynamics McGraw-Hill, 2001.
- 2. M. Mortimer P. G. Tylor Chemical Kinetics and Mechanism Royal Society of Chemistry, 2002.
- 3. G. D. Billing K. V. Mikkelsen, Advanced Molecular Dynamics and chemical Kinetics. Wiley-Interscience, 1997.
- 4. K. J. Laidler, Chemical Kinetics, 3rd edition, Harper and Row, 1987.
- 5. Steinfeld, Francisco and Hase, Chemical Kinetics and Dynamics, Prentice-Hall, 1999.

Credit Hours: 03

Course Title: Chemical and Statistical Thermodynamics

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about principles, laws of chemical and statistical thermodynamics and various theories of statistical thermodynamics. The students will also be able to study the applications of thermodynamics.

COURSE CONTENTS:

1. **INTRODUCTION:** Fundamental concepts, the Zeroth law.

- 2. **ENERGY AND FIRST LAW OF THERMODYNAMICS**: Heat flow, heat capacity and work and heat, Energy as state function, empirical temperature enthalpy energy equation of steady flow, the heat engine and the refrigerator.
- 3. **SECOND AND THIRD LAW OF THERMODYNAMICS:** Entropy, Clausius and Kelvin-Planck statements of the second Law, Helmholtz and Gibb"s function. The third law,
- 4. **STATISTICAL THERMODYNAMICS**: Introduction: Macroscopic and microscopic variables, The Bose-Einstein statistics, The Fermi-Dirac statistics. The Maxwell Boltzmann statistics, Distribution function, Partition function, applications.

- 1. F. W.Sears G. L. Salinger Thermodynamics, Kinetic Theory and Statistical Thermodynamics (3rd Edition)John Wiley, 1975.
- 2. B.N. Roy, Fundamentals of Classical and Statistical Thermodynamics John Wiley, 2002.
- **3.** H.B. Callen Thermodynamics and Introduction to Thermostatistics, 2nd Edition John Wiley, 1985

Credit Hours: 03

Course Title: Advanced Quantum Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the principles and theoretical background of Quantum chemistry, laws and principles and the application of theoretical knowledge of Quantum chemistry in experimental work.

COURSE CONTENTS:

- 1 **Introduction:** Basic principles, wave mechanics, Schrodinger equation.
- 2 **Free/Bound Particles:** Barriers, tunneling, particle-in-a-box.
- 3 **Quantum Mechanics:** Operators, eigenvalue equations, 3-dimensional equations, wave functions.
- 4 **The Harmonic Oscillator:** Solutions, molecular vibration.
- 5 **Angular Momentum:** Commutation relations, angular momentum operators, spherical harmonics, ladder operators, rigid rotor.
- 6 **The Hydrogen Atom:** Separation of variables, energy levels and quantum numbers, wave functions, orbitals.
- 7 **More Quantum Mechanics:** Hermitian operators, basis sets, parity, postulates, matrix formulation
- 8 **Approximations in Quantum Mechanics**: Variational methods, perturbation theory, time-dependent interactions
- 9 **Multi-electron Systems:** Electron spin, Pauli principle, electron interactions
- 10 **Molecular Systems:** Molecular symmetry, Born-Oppenheimer approximation, bonding and electronic structure, molecular orbitals, excited states, MO and VB wavefunctions, dipole moments, virial theorem

11 **Theoretical Quantum Chemistry:** Ab-initio methods, SCF-MO treatment, configuration interaction, perturbation treatments, density-functional theory, semi-empirical methods, Huckel theory, molecular mechanics, computational chemistry.

- 1. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, Oxford, 1996
- 2. D. A. McQuarrie, Quantum Chemistry, University Science Books, 1983
- 3. I.N. Levine, Quantum Chemistry, Prentice Hall, 2000
- 4. J. P. Lowe, Quantum Chemistry, Academic Press, 1993

Credit Hours:

03

Course Title:

ADVANCED MOLECULAR SPECTROSCOPY

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the fundamental and theoretical background of molecular spectroscopy, classification and difference between types of spectroscopy. The contents of the course will enable the students to interpret their experimental findings on the basis of their theoretical knowledge.

COURSE CONTENTS:

- 1 **Introduction:** Radiation and matter, Quantization and molecular energy levels, The intensity of spectral lines, Population and intensity, Selection rules and intensity, Line widths, Stimulated emission, Spontaneous emission.
- 2 **Pure Rotation Spectra:** The rotational energy levels, Spherical top molecules, Symmetric top molecules, Linear molecules, Rotational transitions, Rotational Raman spectra
- 3 **Vibrations of Molecules:** Molecular vibrations, Vibration spectra of diatomic molecules, Vibration-rotation spectra of diatomic molecules, Vibrational Raman spectra of diatomic molecules Vibrational spectra of polyatomic molecules, Vibrational Raman spectra of polyatomic molecules
- 4 **Electronic Spectroscopy, Diatomic Molecules:** The vibrational and rotational structure of electronic bands, Electronic state of atoms, Electronic orbitals and electronic states of diatomic molecules, potential energy curves for electronic states of diatomic molecules.
- 5 **Electronic Spectroscopy, Polyatomic Molecules:** Electronic states of localized groups, Electronic transitions and absorption bands, Conjugated systems by the free-electron model, Electronic states and transition in aromatic systems, Coordination compounds, Nonradioactive processes, Fluorescence
- 6 **Resonance Spectroscopy:** Electron spin resonance, Nuclear magnetic resonance, Mossbauer spectroscopy

- 1. J. M. Brown. Molecular Spectroscopy Oxford, 1998.
- 2. S. Duckett D. B. Gilbert, Foundation of Spectroscopy Oxford, 1999
- 3. C. Banwell E. McCash, Fundamentals of Molecular Spectroscopy McGraw-Hill, 1994
- 4. J. M. Hollans, Modern Spectroscopy John Wiley, 1996
- 5. J. I. Steinfeld, Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy IT Press, 1978

Credit Hours: 03

Course Title: Environmental Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the fundamental principles of environmental chemistry especially related to various environmental pollutions and treatment and management of numerous toxic and hazardous wastes.

COURSE CONTENTS:

- 1 **Introduction:** Environmental chemistry, Environmental segments, Species present in environment, types of pollution, Environmental radioactivity.
- Air Pollution: Classification of air pollution, Acid rain, Photochemical smog, Characteristics of pollutants, Air quality standards, Atmospheric sampling and analysis, Air pollution from industrial and other sources,
- Water Pollution: Types of water pollutants, Organic pollutants, Inorganic pollutants, Physical and chemical characterization of pollutants, waste water treatments, Advanced oxidation technologies (AOT) for water treatment, Wastewater from some typical industries.
- 4 **Solid Pollutants:** Classification and origin of solid wastes, Characteristics of solid wastes, Solid waste treatment and methods of disposal.
- 5 **Toxic and Hazardous Waste:** Types of toxic and hazardous waste, Radioactive waste, Nuclear waste management, Toxic chemicals, Treatment and disposal of hazardous waste, Control and treatment of trace elements.

- 1. S. E. Manahan, Environmental Chemistry, CRC, Florida, 1999.
- 2. C. Baird W. H. Freeman, Environmental Chemistry N.Y., 1994.
- 3. S. S. Dara, A Text Book of Environmental Chemistry and Pollution Control Chand. Co.New Delhi, 1993.
- **4.** S. Chose, Environmental Chemistry Dominant, New Delhi, 2003.

Credit Hours: 03

Course Title: Colloidal Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the principles of colloidal chemistry especially related to electrophoresis, zeta potential, micells, thermodynamics and applications of colloides.

COURSE CONTENTS:

- 1 **Colloidal Materials:** Basic concepts, Preparation techniques, Characterization, brownian motion and flocculation.
- 2 Colloidal Forces: Basic concepts of interfaces, Vander walls, Double layer and other short range forces, Thermodynamics of interfacial tensions and two dimensional equation of states. Stability of colloidal dispersions. Dl Vo Theory
- 3 **Electrokinetic Phenomena:** Electrophoresis, Zeta Potential measurement and applications.
- 4 **Colloidal Association:** Micells, Micillar thermodynamics and micellar applications.

- 1. P.c. Hiemenz, R. Rajagopalan, Principles of Colloidal and Surface Chemistry, Dekker, New York, 1997.
- 2. A.W. AdamsonA. Gast, Physical Chemistry of Surfaces J. Wiley, 1999.
- 3. D. F. Evans, H. Wennerstrom, The Colloidal Domain: Where Physics, Chemistry, Biology and Technology Meet. VCH New York, 1194.
- 4. R. J. Huntetr, Foundation of Colloid Science, Volume I., Oxford science, Oxford. 1989
- 5. W. B. Russel, D. Saville, W. Schowalter, Colloida; Dispersions, CambridgeUniversity Press, Cambridge, 1989

Credit Hours: 03

Course Title: Polymer Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the fundamentals of polymer chemistry, polymer synthesis, characterization and thermal and mechanical properties of polymers. The students will also be able to study polymer degradation and their environmental impacts.

COURSE CONTENTS:

- 1. **Introduction:** The Science of large molecules, basic concepts of polymer science, History of macromolecular science, molecular forces and chemical bonding in polymers.
- 2. **Polymer Synthesis:** Step Growth polymerization, Free Radical Chain Polymerization Ionic, Polymerization, Co-polymerization, emulsion polymerization.
- 3. **Characterization of polymers:** Dissolution of polymers, Solubility parameters, Entropy of mixing. End Group Analysis, Colligative property, Measurement, Light Scattering, Solution viscosity, Ultracentrifugation.
- 4. **Thermal and Mechanical Properties of Polymers:** The Glass Transition Temperature (Tg), Methods of determining the Tg, Viscoelastic state, linear viscoelastic behaviour of amorphous polymers, Time-Temperature superposition Principle.
- 5. **Structure Property Relationship:** General consideration, Control of Tm and Tg, Plasticizers, Crystallinity and Mechanical response, Applications to fibers, elastomers and plastics.
- 6. **Special topics in Polymer Chemistry:** Polymer Liquid Crystals, Polymers in Electronic Industry, Polymer composites and Blends, Polymers and Environment, High Temperature specialty polymers, Poly electrolytes, Polymers for food packaging Degradable polymers.

- 1. J.MN.G. Cowie, Polymers: chemistry and Physics of Modern Materials (2nd Edition)Blackie glasgow, 2001.
- 2. George Odian, Principles of Polymerization (2nd edition), John Wiley (1981).
- 3. R.B. Seymour, C.E. Carraher, Polymer Chemistry Marcel Deckker, 2000.
- 4. R. Sheldon, Composite Polymeric Materials Applied Science, 1982.

Credit Hours: 03

Course Title: Heterogeneous Catalysis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the principles of heterogeneous catalysis, classification, kinetics of catalytic reactions and industrially useful catalytic reactions.

COURSE CONTENTS:

- 1. **Introduction:** Historical, Definition of catalysis, The basis of catalytic action, Requirement of an industrially useful chemical reaction, Kinetics of catalyzed reaction, Implication of the definition of catalysis, Catalysts in action, Classification of catalytic systems, Classification of solid catalysts.
- 2. **Adsorption on Solid Surfaces:** Adsorption of molecule at solid surfaces, Adsorption isotherms, Surface area and porosity.
- 3. **Chemisorption at Metal Surfaces:** Metal surface for fundamental research, Adsorbed states of molecules on metals, Potential-energy curves for adsorption, Descriptive chemistry of chemisorption on metals, Quantitative aspect of chemisorption on metals.
- Chemisorption at Oxide Surfaces: Introduction, Electrical conductivity of solids, The Band Theory of solids, Chemisorption at semi conducting oxides, Adsorption on insulator oxides.
- 5. **Kinetics of Catalyzed Reactions:** Rates and order of reactions, Effect of temperature on the rates of catalyzed reactions, Mass-transport limitation of catalyzed reactions.

- M. Bowker, Basics and Application of Heterogeneous Catalysis Oxford, 1998
- 2. B.C. Gates, Catalytic chemistry John Wiley, 1992
- 3. G.C.Bond, Heterogeneous Catalysis: Principals and applications, Oxford, 1987

4. M. Boudart and G.D. Mariadassou, Kinetics of Heterogeneous catalytic reactions, Princeton, 1984.

DISSERTATION/RESEARCH/SEMINAR

Course Code: CH-790

Credit Hours: 06

Course Title: Research

The student has to conduct research on specific topic under supervision of faculty member.

Thesis

The student shall submit a thesis on the subject of his/her research work for evaluation and an oral examination.

Seminar on Research / Thesis

The student shall give a seminar on the topic of his/her research.

PHD COURSES

ANALYTICAL CHEMISTRY

Course Code: CH-801

Credit hours: 03

Course Title: Nano Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of nanomaterials. The course will enable the students to design synthesis of new nanomaterials and their analysis and characterization.

COURSE CONTENTS:

Nanotechnology, nanomaterials, mesoporous, microporous and macroporous materials. Nanometer, Nanoparticles, Nanotubes, Thin films, Nanoscale, Nanocomposites, Nanostructured bulk materials. Synthesis of nanoparticles, mesoporous materials and composites (Bottom Up and Top Down Production). Synthesis by anodization, hydrothermal, convention heating, deposition-precipiation methods. Characterization of nanomaterials by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Brunauer, Emmett and Teller (BET) adsorption method, Thermogravimetric Analysis (TGA), Atomic Absorption Spectroscopy (AAS), Ultraviolet-Visible Spectroscopy (UV-Vis) and Fourier Transform Infrared (FTIR) spectroscopy etc. Importance of nanotechnology with special reference to environmental pollution, gas sensors, solar cells, catalysis. Size dependent properties of nanomaterials, structure, bonding, Specific heat and melting points of nano-crystalline materials, Chemical and catalytic aspects of nanocrystals. Semiconductor nanocrystals, Spinels, quantum dots. Alloy semiconductors and their synthesis. Metal nanoparticles. Nanoparticle stability. Optical properties, Magnetic Properties, Magnetic anisotropy, Magnetic domains, Hysteresis, Langevin model, quantum effects, Curie-Weiss law. Nanotechnology: Synthesis techniques. Applications of nanomaterials.

RECOMMENDED BOOKS:

1. KJ. Klabunde, Nanoscale Materials in Chemistry, John Wiley, New York (2001).

- 2. D. Jiles, Introduction to Magnetism and Magnetic Materials, Nelson Thomes, Cheltenham (1998).
- 3. C.C. Koch, Nanostructured Materials, Processing, Properties and Potential Applications, William Andrew Publishing, New York (2002).
- 5. M. Schwartz, New Materials, Process, and Methods Technology, CRC Press, New York (2006).
- 7- Augus I Kirkland and John L Hutchison "Nanocharacterisation" The Royal Society of Chemistry, UK (2007).
- 9- Hideo Hosono, Kenneth MacKenzie, YoshinaoMishima, Hideo Takezoe, 'Nanomaterials' Elsevier Science Ltd, (2006)

Credit hours: 03

Course Title: Nuclear methods of Analysis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the nuclear methods of analysis that will be useful during the characterization of newly synthesized compounds.

COURSE CONTENTS:

Fundamentals of radiochemistry, specific applications of nuclear techniques to analytical chemistry including radioimmunoassay and activation techniques using very short-lined indicator adionuclides, Current nuclear methods of analysis such as neutron activation PIXE, nuclear reaction analysis, Rutherford backscattering, isotope dilution analysis and others.

- 1. William D. Ehmann, Diane E. Vance, radiochemistry and nuclear methods of analysis, Wiley publishers
- 2. Walter D. Loveland, David J. Morrissey, Glenn Theodore Seaborg, Modern Nuclear Chemistry, Wiley publishers Instrumental Analysis by Skoog and Crouch Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Principles of Instrumental Analysis, 6th edition, Thomson Brooks/Cole.

Credit Hours: 03

Course Title: Advanced Chromatographic Techniques

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the advanced methods of chromatography. The course will enable the students to carry out synthesis efficiently.

COURSE CONTENTS:

Introduction to chromatographic techniques: Principles of chromatographic separation. Conventional chromatographic techniques: Paper, thin layer, and column chromatography. Pressure chromatographic techniques: High performance, medium pressure, high pressure thin layer liquid, vacuum liquid, flash, centrifugal thin layer and gas chromatography. Liquid-liquid chromatography techniques, Paper electrophoresis, capillary zone electrophoresis. Gas chromatography, mass spectrometry and liquid chromatography-mass spectrometry. Application of chromatographic techniques: Separation of various substances.

- 1. K. Hosttetman, A. Marston and M. Hostettmann, Preparative chromatography Techniques, Springer (1997).
- 2. W.M.A Niessen and J. Van der Greef, Liquid Chromatography-mass spectrometry: principles and applications, Marcel Dekker, New York (1992).
- 3. H.M. McNair and J.M. Miller, Basic Gas Chromatography, John Wiley & Sons, Inc. (1998).
- 4. D. Hage, Handbook of Affinity Chromatography, Hage David Saylor & Francis, Inc. (2005).
- 5. B. Kolb and L.S. Ettre, Static Headspace-Gas Chromatography: Theory and Practice, Wiley, John & Sons, Inc. (2006).
- 6. P.R. Brown, Advances in Chromatography, Vol. 41, E. Grushka (Ed.), Marcel Dekker (2001).

- 7. P.R. Brown, Advances in Chromatography, Vol. 40, E. Grushka (Ed.), Marcel Dekker (2000).
- 8. P.R. Brown, Advances in Chromatography, Vol. 37, E. Grushka (Ed.), Marcel Dekker (1997).
- 9. R.E. Ardrey, Liquid Chromatography Mass Spectrometry: An Introduction, John Wiley & Sons (2003).

Credit Hours: 03

Course Title: Molecular Spectroscopy

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the spectroscopy at molecular level useful in the characterization of newly synthesized materials.

COURSE CONTENTS:

Introduction of molecular spectroscopy; Electronic spectroscopy: Ultraviolet and visible basic principles, Introduction to theories of molecular bonding; classification of molecular orbitals and electronic transitions; selection rules; absorption of radiation, effect of structure on absorption, quantitative absorption spectroscopy, electronic spectra of diatomic and simple polyatornic molecules; dissociation and dissociation products; and applications towards analytical chemistry. IR spectroscopy and spectral interpretation. Raman spectroscopy: Principles; applications to diatomic and simple molecules. Molecular fluorescence basic theory, instrumentation and analytical applications. Effect of chemical and environmental factors on fluorescence efficiency, phosphorescence, instrumentation and applications.

- 1. C.N. Banwell, Fundamentals of Molecular Spectroscopy, 3rd ed., McGraw-I-till, UK (1983).
- 2. J.D. Graybeal, Molecular Spectroscopy, International Edition, McGraw-Hill Book Company, New York (1988).
- 3. J.MiIollas, High Resolution Specroscopy, 2 ed., Wiley, USA (1998).
- 4. Robert D. Braun, Introduction to Instrumental Analysis McGraw Hill Book Co. New York.
- 5. Gary D. Christian, James E. O'Reilly, Instrumental Analysis, Allyn and Bacon Inc. New York.
- 6. Douglas A. Skoog, Stanley R. Crouch, Instrumental Analysis, Reinholt, New York.
- 7. F.W. Fifield and D. Kealy, Principles and Practice of Analytical Chemistry I.T.B, London.

- 8. Willard, Meritte and Dean, Instrumental Analysis, D. Van Nostrand, New York.
- 9. Bernhard Wetz, Atomic Absorption Spectroscopy, VerlayChemie, New York.

Credit Hours: 03

Course Title: Advanced Analytical Instrumental Techniques

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the advanced instrumental techniques apart from conventional methods.

COURSE CONTENTS:

Principles of mass spectrometry and gas chromatography, instrumentation, application of mass spectrometry to organometallics, organosilicon and organophosphorus compounds. Mass spectrometry coupled with gas chromatography. Discussion on relevant research papers and review articles.

- 1. D.A. Skoog, Principles of Instrumental Analysis, 3rd ed., Saunder College Publishing, Philadelphia (1984).
- 2. G.W. Ewing, Instrumental Methods of Chemical Analysis, McGraw-Hill, New York (1985).
- 3. D.A. Skoog, et al., West and Holler, Fundamentals of Analytical Chemistry Office, 8th ed., Thomson, Brooks/Cole, Australia (2004).

Credit Hours: 03

Course Title: Advanced Thermal Analysis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the modern methods of thermal analysis used during the characterization of compounds. The course will enrich the students with modern sophisticated thermal analytical techniques.

COURSE CONTENTS:

Theory and instrumentation: Thermogravimetry (TG), differential thermal analysis (DTA), differential scanning calorimetry (DSC). Quantitative interpretation: TGA, DTA and DSC curves. Kinetic and thermodynamic parameters. Applications: DTA, TGA in cements, catalysts, clays, minerals, biological materials, drugs, polymers and textiles. High temperature reflectance spectroscopy (HTRS): Instrumentation and applications to various inorganic compounds.

- 1. T. Hatakeyama and F.X. Quinn, 2nd ed., Thermal Analysis Fundamentals and Applications to Polymer Science, John Wiley, New York (1999).
- 2. P.J. Haines, Thermal Methods of Analysis, Blackie Academic and Professional, London (1995).
- 3. W.W.M. Wendlandt, Thermal Analysis, 3rd ed., John Wiley, New York (1986).
- 4. T. Daniels, Thermal Analysis, Kogan Page, London (1973).
- 5. J.W. Dodd and K.H. Tonge, Thermal Method: Analytical Chemistry by Open Learning, John Wiley (1987).

Credit Hours: 03

Course Title: Advanced Chemometrics

COURSE LEARNING OBJECTIVES AND OUTCOMES:

The course introduces advanced chemometric methods and their use on different kinds of multivariate data of relevance for research and development. After completing the course the student should be able to Summarize basic chemometric methods, Describe advanced chemometric methods for multivariate (clustering, classification and regression) data analysis, Describe advanced techniques for data prepreprocessing, Describe advanced methods for variable selection, Apply theory on real life data analytical cases, Apply commercial software for data analysis, Report in writing a full data analysis of a given problem including all aspects presented under Knowledge, Discuss advantages and drawbacks of advanced methods

COURSE CONTENTS:

Advanced Preprocessing for Spectroscopic Applications

- Preprocessing Objectives
- Mean- and Median-centering, Autoscaling
- Normalization and Standard Normal Variate Scaling
- Scaling for Multi-block data
- Savitsky-Golay and Filtering
- Multiplicative Scatter Correction (MSC)
- External Parameter Orthogonalization (EPO)
- Extended Multiplicative Scatter Correction (EMSC)
- Generalized Least Squares and GLS-like Weighting
- Orthogonal Signal Correction (OSC) and Orthogonal-PLS

Variable Selection

- Motivation and Preliminary Examples: Why select variables?
- Available Variable Selection Methods:
- A priori
- A posteriori
- Model based, e.g. on loadings

- Genetic algorithms
- Classical
- Forward, backward selection
- Best subset selection
- Significance tests
- Significance based on Jack-knife
- i-PLS
- How to choose a variable selection method
- Variable selection in practice

Calibration Model Maintenance

- Introduction to Model Maintenance
- Goals
- Causes of data/model mismatch
- Identifying the need for action
- External validation samples
- Model prediction diagnostics Q and T^2
- Setting action limits
- Determining the source of the problem
- Model updating methods
- Slope and bias adjustments
- Adding to the calibration set
- Automatic model updating
- Instrument standardization methods
- Direct and Piecewise Direct standardization
- Spectral Subspace Transformation
- Filtering approaches: GLS and OSC
- Avoiding model updating
- Preprocessing methods that tend to make model more brittle
- Using the model robustness tests

Chemometrics in Metabolomics

- Introduction to metabolomics
- What is metabolomics?
- Which kind of measuring techniques are used?
- What kind of preprocessing is needed?

- What kind of data does it generate and how does this differ from 'normal' chemometric data?
- Practical examples of metabolomics
- Biomedical sciences: biomarkers for disease and challenge tests
- Biotechnology: metabolic engineering and synthetic biology
- Nutritional sciences: nutrikinetics
- Practical examples from metabolomics, food quality and process analytical technology

Modeling Fluorescence EEM Data

- Introduction to fluorescence EEM spectroscopy
- The structure of fluorescence data
- The PARAFAC model
- Validating and using the PARAFAC model
- Handling Rayleigh scatter
- Handling Raman scatter
- Handling inner filter effects

Robust Methods

- The outlier problem
- Robust estimation of the mean: Median
- Robust estimation of the covariance matrix: Minimum Covariance Determinant
- Robust linear regresssion
- Robust Principal Components Analysis: ROBPCA
- Robust Regression in High Dimensions: ROBPCR and ROBPLS

Practical & Tutorials

- Spectroscopic & Chemometric studies of edible date fruits growing in Sultanate of Oman
- Detection and Estimation of Super premium 95 gasoline adulteration with Premium 91 gasoline using new NIR spectroscopy combined with Multivariate Methods
- Development of Near Infrared spectroscopic methods combined with Chemometrics for physiochemical characterization of hydrocarbon fuels, which are derived or synthesized from petroleum or biomass
- Identification of Protein Biomarkers in Halal Meat using proteomics and Reflectance Infrared spectroscopy coupled with chemometrics
- Robust reflectance spectroscopy (FTIR-ATR, NIR): A diagnostic tool for detection of infectious diseases & biomarker identification in clinical samples
- New robust Infrared spectroscopy (FTIR-ATR, NIR) coupled with multivariate methods for detection
 & quantification of pesticides residue plants, soil and blood samples
- Applications of reflectance spectroscopies (FTIR-ATR & NIR) as a tool for robust detection & quantification of pork gelatin adulteration in other processed food samples

- New robust sensitive fluorescence spectroscopy coupled with PLSR for estimation of quercetin in Ziziphus mucronata and Ziziphus sativa
- Fluorescence spectroscopy-partial least square regression method for the quantification of quercetin in Euphorbia masirahensis.

RECOMMENDED BOOKS / MATERIALS / REFERENCES:

- 1. http://www.eigenvector.com/training.htm
- 2. https://www.camo.com/unscrambler/
- 3. Introduction to Multivariate Statistical Analysis in Chemometrics, Kurt Varmuza, Peter Filzmoser, CRC Press, 2009.
- 4. Multivariate Statistics, Hardle, Springer Science+Business Media, LLC, 2007.
- 5. Multivariate Data Analysis, Josep FH JR, 7th ed., Elsevier Inc, 2010.
- 6. Applied Multivariate Statistical Analysis, Richard A. Johnson, Dean W. Wichern, 6th ed., Pearson Education Inc, 2007.
- 7. Theory of Multivariate Statistics, Martin Bilodeau, David Brenner, Springer Media New York, 1999.
- 8. Linear Model Theory Univariate, Multivariate, and Mixed Models Wiley Series in Probability and Statistics, Keith E. Muller, Paul W. Stewart, A JOHN WILEY & SONS, INC., PUBLICATION, 2006.
- 9. Multivariate Data Analysis, Hair J.F., Black W.C., Babin B.J., Anderson R.E. 2010.
- 10. Applied Multivariate Data Analysis- Regression and Experimental Design, J. D. Jobson, Springer Science+Business Media New York, 1991.
- 11. Measurement and Multivariate Analysis, John C. Gower, Springer, 2002.
- 12. Regression Linear models in statistics, Bingham N., Fry J., Springer-Verlag London Limited, 2010.

Credit Hours: 03

Course Title: Applications of Polymer Nanofibers

COURSE LEARNING OBJECTIVES AND OUTCOMES:

The course presents a fulsome analysis of the technology of electrospinning, the most convenient and scalable

technique for nanofiber production. It also provides with information on relevant surface modification

Applications of Polymer Nanofibers delivers a complete introduction to the basic science of polymer nanofibers

as well as a review of their diverse applications. This course assesses their potential for commercialization and

presents contributions from leading experts emphasizing their practical and technological details. New and up

to date research findings are presented throughout this course in areas including filters, fabric, sensors, textile

applications aerogels.

COURSE CONTENTS:

Electrospinning Parameters and Resulting Nanofiber Characteristics: Theoretical to Practical

Considerations

Electrospinning Overview, Effect of Process Parameters, Theoretical Analysis, Experimental Results, Effect of

Setup Parameters, Effect of Solution Parameters, Polymer Solution Properties (Molecular Weight,

Concentration, Viscosity, and Elasticity), Solvent Selection, Additivities to Tune Solution Properties, Surface

Tension, Conductivity, Electrospinnable Systems, Nonpolymer Electrospinning, Advanced Fiber

Characteristics, Ribbons, Wrinkles, Branching, and Netting, Porous Fibers, Core-Shell Fibers, Coaxial

Electrospinning, Emulsion Electrospinning, Process Scalability, Melt Electrospinning, Needleless or "Free-

Surface" Electrospinning, Alternative Fiber Production Methods

Textile Applications of Nanofibers

Introduction of Nanofibers in Textile Applications, Fabrication of Nanofiber Yarns, Electrospinning,

Bicomponent Spinning, Melt Blowing, Flash Spinning, Centrifugal Spinning, Formation of Nanofiber Yarns,

Structure and Properties of Nanofiber Yarns, Fabrication of Nanofiber Fabrics, Nanofibrous Nonwoven Fabrics,

Nanofibrous Woven Fabrics 54, Characteristics and Specialized Applications of Nanofiber Fabrics, Protective

Clothing, Filter Fabrics, Wearable Devices, Functional Fabrics, Biomedical Textiles, Summary and Future

Trends

Nanofiber-Based Chemical Sensors

Introduction, General Features of Sensors, Nanofibers as a Sensor Material, Nanofiber vs. Thin-Film Geometry,

Approaches to Nanofiber Sensor Design, Gravimetric Nanofiber Sensors, Quartz Crystal Microbalance, Surface

Page | 75

Acoustic Wave Resonators, Optical Sensors, Colorimetric Sensors, Fluorescence Sensors, Electrochemical Sensors, Metal-Oxide Sensors, Graphene-Based Sensors

Nanofiber Aerogels: Bringing a Third Dimension to Electrospun Nanofibers

Aerogels, Processing, Properties and Applications, Challenges, Nanofiber-Based Aerogels, Historical Background, Fabrication of Nanofiber-Based Aerogels (NFAs), Electrospinning, Dispersion Preparation, Solid Templating, Applications, Filtration, Thermal Insulation, Building and Lightweight Construction, Future Perspectives

Micro and Nanofibers

Electrospinning, The Melt-blowing Process, The Reicofil Process, The Biax Multirow Process, The Hills Process, "Splittable" Bicomponent Fibers, Partially "Soluble" Bicomponent Fibers, Fibrillating Bicomponent Fibers

- 1. "Polymer Nanofibers: Building Blocks for Nanotechnology" by Sajjad Haider and Abbas Hamrang. [Reference: ISBN 978-3527338238]
- 2. Electrospinning for Advanced Energy and Environmental Application" edited by Jingwei Xie, Mahmood Ali of khazraei, and Ali Saberi. [Reference: ISBN 978-1119128105]
- 3. Polymer Nanofibers: Fabrication, Characterization and Applications" edited by Amit Rawal. [Reference: ISBN 978-1498749384]
- 4. "Nanofiber Composited Materials: Techniques, Manufacturing and Applications" edited by Jitendra S. Tate and Klaus Friedrich. [Reference: ISBN 978-3527344147]
- 5. "Electrospinning: Principles, Practice and Possibilities" by Geoffrey R. Mitchell. [Reference: ISBN 978-1856175354]

INORGANIC CHEMISTRY

Course Code: CH-821

Credit Hours: 03

Course Title: Advanced Nuclear and Radiation Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students would get knowledge about sources of nuclear radiations, tracers, etchants, kinetics of radioactive decay processes, dosimeters, radiaolysis and radiobiology concepts.

COURSE CONTENTS:

Nuclear Chemistry: Introduction to the nuclear Chemistry, Sources of nuclear radiations, Nuclear track detectors, Etchants, Mechanism of track etching, Nuclear materials, Tracers, Applications of Tracers in Chemistry, Nuclear fission and fusion, Nuclear hazards and their prevention. Radiation Chemistry: Theoretical aspects, Interaction of ionizing radiation with matter, Kinetics of radioactive decay processes, Radioactive decay series, Production of ionization and excitation, Linear energy transfer (LET), Kinetic studies of radiolytic processes, Radiation dosimetry (physical and chemical), Various types of radiation dosimeters, Radiation chemical yields, Dose and dose rate effect on the primary and secondary products, Radiolysis, Pulse radiolysis technique, Radiolytic studies of gaseous, aqueous and organic systems, Radiobiology.

- 1. Choppin, G. and J. Rydberg. 2001. Nuclear Chemistry, theory and applications. 1st Ed., Pergamon Press, New York, USA.
- 2. Friedlander, G., J. W. Kennedy, E. S. Macias J. M. Miller. 1981. Nuclear and Radiochemistry. 3rd Ed., John Wiley and Sons, New York, USA.
- 3. Levine, I. N. 2008. Physical Chemistry. 6th Ed. McGraw Hill New York.
- 4. Mozumder, A. 2004. Fundamentals of Radiation Chemistry. Academic Press, UK.
- 5. Satake, M. and Y. Mido. 1995. An introduction to Nuclear Chemistry. Discovery Publishing House New Delhi.
- 6. Spinks, J. W. T. and R. J. Woods. 1990. An introduction to Radiation Chemistry. 3rd Ed, John Wiley and Sons, New York, USA.

7. Goplan, R. 2000. Elements of Nuclear Chemistry. Vikas Publishing House New Delhi.

03

Credit Hours:

Course Title: Organo-transition Metal Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of organotransition metal compounds. The course will enable the students to carry out synthesis of the complexes.

COURSE CONTENTS:

Classification of organometallic compounds; transition metal to carbon sigma bonded compounds, complexes with metal-carbon pi bonds such as $\eta 2-\eta 7$. Synthesis, properties and nature of bonding in pi complexes. Complexes of molecular nitrogen, oxygen and carbon disulphide. Fundamental processes in organometallics, fluxional and dynamic equilibrium, oxidative addition and reductive elimination, insertion and deinsertion, reactions of coordinated ligands. Catalysis by oraganometallic (stoichiometric and catalytic processes) compounds. Polymerization and oligomerization, synthesis with COhydrogenation of olefin etc.

- 1. A. Yamamoto, Organotransition Metal Chemistry Fundamental Concepts and Applications, John Wiley & Sons (1986).
- 1. M.L.H. Green, G.E. Coates and K. Wades, Organometallic Compounds, Methuen & Co. Ltd., (1968).
- 2. M. Bochmann, Organometallic 1 and 2, Oxford Science Publications (1994).
- 3. F.A. Cotton, G. Wilkenson, Advanced Inorganic Chemistry, 6th Ed. John Wiley & Sons, (1999).

Credit Hours:

03

Course Title: Bio-Inorganic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of bio-inorganic compounds. The course will enable the students to design synthesis of new bio-inorganic compounds.

COURSE CONTENTS:

Introduction: Development and importance of bio-inorganic chemistry. Metals and Complexes: Metals of biological importance. Function of metals in enzyme catalysis. Metalloproteins and enzymes containing a transition metal center at their active site. Oxygen carriers; uptake and transport activation and utilization; synthetic dioxygen carriers; nitrogen fixation; vitamin B6 and B12. Importance of nonmetals in biological systems. Metal ions and chelating agents in biological systems.

- 1. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Corporation, New Delhi (1997).
- 2. R.W. Hay, Bioinorganic Chemistry, Ellis Horwood, London (1984).
- I. Bertim, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, Viva Book Private Ltd. New Delhi (1998).
- 3. B.K. Keppler, Metal Complexes in Cancer Chemotherapy, VCH, Weinheim (1993).
- 4. M.F. Gielen, Metal Based Anti-tumor Drugs, Freund Publishing House Ltd. London (1988).

Credit Hours: 03

Course Title: Catalysis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of catalysts. The course will enrich the students to use the catalyst efficiently and design synthesis of new catalysts.

COURSE CONTENTS:

Physical adsorption, Chemisorption of gases on metals and metal oxides, textural and structural characterization of catalysts, Synthesis of porous solids, Kinetics of catalytic reactions, Catalysis and theoretical concepts, Catalytic process such as oxidation reactions, production of petrochemicals, environmental catalysis, polymerization and photocatalysis, Catalyst deactivation, Fuel cells.

- 1. B. Viswanath, S. Sivasanker and A.V. Ramaswamy, Catalysis Principles and Applications, Narosa Publishing House, New Delhi, India (2006).
- 2. J. Hagen, Industrial Catalysis: A Practical Approach, 2nd rev. ed., Wiley-VCH, Weinheim, Germany (2006).
- 3. R. Richards, Surfaces and Nanomolecular Catalysis, CRC, Taylor/Frances, Boca Raton (2006).
- 4. K. Bucholz and V. Kasche, Biocatalysis and Enzyme Technology, Wiley-VCH, New York (2005).
- 5. Chorkendorff and J.W. Niemantsverdriet, Concepts of Modern Catalysis and Kinetics, Wiley-VCH, Weinheim, Germany, New York (2003).
- A. Weichkowski et al., Catalysis and Electrocatalysis at Nanoparticles Surfaces, Marcel Dekker, New York (2003).
- 6. S. Bhaduri and D. Mukesh, Homogenous Catalysis: Mechanisms and Industrial Applications, John Wiley-Interscience, New York (2000).
- 7. J. Tsuji, Transition Metal Reagents and Catalysis: Innovation in Organic Synthesis, John Wiley and Sons, Chichester/New York (2000).

- 8. S.M. Robert, Biocatalysts for Fine Chemical Synthesis, John Wiley and Sons, Chichester (1999).
- 9. Bond, Heterogeneous Catalysis: Principles and Applications, Clarendon Press, Oxford (1986).
- 10. J.M. Thomas and R.M. Lambert (Eds.), Characterization of Catalysis, John Wiley & Sons, Chichester (1980).

ORGANIC CHEMISTRY

Course Code: CH-841

Credit Hours: 03

Course Title: Modern Name Reactions in Organic Synthesis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about different named organic reactions that are used in the current organic research work. The course will be helpful in

the designing the synthesis of new and novel important compounds.

COURSE CONTENTS:

Recent modifications and advancements in classical name reactions: Evans Aldol

Condensation, Mukaiyama Aldol, Barton-McCombie Reaction, Baylis-Hillman Reaction,

Biginelli Reaction, Bishler-Napieralski Reaction, Blanc Reaction, Brook Rearrangement,

Castro-Stephens Coupling, Cory-Kim Oxidation, Dakin-West Reaction, Hetero-Diels-Alder

Reaction, Eschenmoser Fragmentation, Friedlander Synthesis, Horner-Wadsworth-

Emmons reaction, Milas Hydroxylation Reaction, Pictet-Spengler Ritter Reaction, Doebner

Modification.

Recent name reactions and their application: Sharpless Dihydroxylation, reactions, CBS

reduction, Dess-Martin Oxidation, Swern Oxidation, Stephen aldehyde synthesis, Corey-

Fuchs reaction, Fukuyama, Sonogashira, Stille Suzuki, McMurry and Heck coupling, Ugi

reaction, Wittig Rearrangement, Mitsunobu Reaction, McMurry coupling, Fujimoto-Belleau

reaction, Tebbe olefination, Tamao oxidation, Weinreb synthesis.

RECOMMENDED BOOKS:

1. L. Kurti and B. Czako, Strategic Applications of Name Reactions in Organic Synthesis,

Academic Press, New York (2005).

2. L. Kurti and B. Czako, Name Reactions and Reagents in Organic Synthesis, 2nd ed.,

Elsevier, Amsterdam (2005).

3. B. P. Mundy, M. G. Ellerd, et al., Name Reactions and Reagents in Organic Synthesis,

John Wiley, New York (2005).

SUPPLEMENTARY BOOKS:

Page | 83

- 1 T. Laue and A. Plagens, *Name Organic Reactions*, John Wiley and Sons: Chichester, England, New York (1998).
- 2 J. J. Li, Name Reactions: A Collection of Detailed Reaction Mechanisms, 3rd ed., Springer-Verlag, Berlin (2006).

Credit Hours: 03

Course Title: Computational Chemistry/Molecular Modeling

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the computational chemistry and molecular modeling. The course will be helpful in understanding the different aspects of organic compounds.

COURSE CONTENTS:

Basic concepts: Wave function and Schrödinger wave equation, probability distribution of wave function. Molecular mechanics: Single point energy calculations, geometry optimization and molecular modeling. Semiempirical and ab initio molecular orbital methods: Prediction of molecular properties, spectra and reactivity of organic compounds. Molecular docking and QSAR: Use of available software packages e.g., Hyperchem and Gaussian for MO calculations, MOE and Autodock for QSAR and molecular docking.

RECOMMENDED BOOKS:

- 1. A. Hinchcliffe, Modelling Molecular Structures, John Wiley and Sons, England (2000).
- 2. H.J. Cremer, Essentials of Computational Chemistry, 2nd ed., Theories and Models (2004).

- 1. A. Frisch and J.B. Foresman, *Exploring Chemistry with Electronic Structure Methods* (*Paperback*), Gaussian Publishers (1993).
- 2. A.R. Leach, Molecular Modelling: Principles and Applications, Prentice Hall (2001).
- 3. A.K. Rappé and C.J. Casewit, *Molecular Mechanics across Chemistry*, University Science Books, Sausalito CA (1997).

03

Credit Hours:

Course Title: Protecting Groups in Organic Synthesis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the concept of protecting groups. The course will be helpful in designing a successful organic synthesis.

COURSE CONTENTS:

Introduction: characteristics of good protecting groups. Protection of various functional groups: Hydroxyl, thiols, carbonyl, amino and carboxylic groups. Synthetic applications: Protection and deprotection of the various functionalities in organic synthesis including peptide bond formation.

RECOMMENDED BOOKS:

- 1. P.J. Kociennski, *Protecting Groups*, George Thieme Verlag, Stuttgart Germany (2003).
- 2. A.J. Person and W.R. Roush, *Activating Agents and Protecting Groups*, John Wiley and Sons, New York (1999).
- 3. T.W. Greene and P.G.M. Wuts, *Protective Groups in Organic synthesis*, John Willey and Sons New York (1999).

SUPPLEMENTARY BOOKS:

1. J.R. Hanson, Protecting Groups in Organic Synthesis, Blackwell Science Ltd. (1999).

Credit Hours: 03

Course Title: Physical Organic Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the different physical aspects of organic compounds and applying this concept to the newly designed and synthesized organic compounds.

COURSE CONTENTS:

History and development: Evolution of a hybrid discipline, energy changes during chemical reactions, theory and principles related to kinetics and equilibrium processes. **Correlation of structure and reactivity:** Hammett equation and other linear free energy relationships. **Hückel molecular orbital (HMO) method:** Correlation of HMO parameters with molecular properties, alternant and nonalternant hydrocarbons and their properties. **Correlation of structure and activity:** Use of molecular descriptors, Hansch analysis, Craig plots, Topliss scheme in establishing SAR. **FMO method:** Concept of Frontier orbitals and its application for explaining chemical reactivity.

RECOMMENDED BOOKS:

- 1. Miller, Advanced Mechanisms in Organic Chemistry, Pearson Education (2004).
- 2. T.H. Lowry and K.H. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd ed., Harper & Row Publisher (1987).
- 3. N.S. Issacs, *Physical Organic Chemistry*, Longman Group (1995).
- 4. A. Streitwieser, Jr., *Molecular Orbital Theory for Organic Chemists*, Wiley, New York (1961).

- 1. E.V. Anslyn, *Modern Physical Organic Chemistry*, University Science Books, US (2006).
- 2. F.L. Ansari, R. Qureshi and M.L. Qureshi, *Electrocyclic Reactions-from Fundamentals* to Research, Wiley-VCH (1999).

- 3. C. Hansch and A. Leo and D.H. Hoekman, *Exploring QSAR:Fundamentals and Applications in Chemistry and Biology*, ACS (1995).
- 4. A. Pross, Theoretical & Physical Principles of Organic Reactivity, Wiley Interscience (1995).

Credit Hours: 03

Course Title: Advances in Chromatographic Techniques

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the conventional and modern chromatographic techniques.

COURSE CONTENTS:

Introduction: Principles of chromatographic separation. Conventional chromatographic techniques: Paper, thin layer, and column chromatography. Pressure chromatographic techniques: High performance-, medium pressure-, high pressure thin layer liquid-, vacuum liquid-, flash-, centrifugal thin layer- and gas chromatography. Liquid-liquid chromatography: Droplet counter current, counter current distribution, and rotation locular counter current chromatography. Miscellaneous chromatographic techniques: Paper electrophoresis and capillary zone electrophoresis. Hyphenated chromatographic techniques: Gas chromatography- mass spectrometry and liquid chromatography-mass spectrometry. Application of chromatographic techniques: Separation of natural products and mixtures of other organic compounds.

RECOMMENDED BOOKS:

- 1. K. Hosttetman, A. Marston and M. Hostettmann, *Preparative chromatography Techniques*, Springer (1997).
- 2. Richard J. P. Cannel (editor), *Natural products isolation*, Humana press, New Jersey, USA (1998).
- 3. W.M.A Niessen and J. Van der Greef, *Liquid Chromatography-mass spectrometry:* principles and applications, Marcel Dekker, New York (1992).

SUPPLEMENTARY BOOKS:

1. H.M. McNair and J.M. Miller, *Basic Gas Chromatography*, John Wiley & Sons, Inc. (1998).

- 2. D. Hage, *Handbook of Affinity Chromatography*, Hage David Saylor & Francis, Inc. (2005).
- 3. B. Kolb and L.S. Ettre, *Static Headspace-Gas Chromatography: Theory and Practice*, Wiley, John & Sons, Inc. (2006).
- 4. P.R. Brown, *Advances in Chromatography*, Vol. 41, E. Grushka (Ed.), Marcel Dekker (2001).
- 5. P.R. Brown, *Advances in Chromatography*, Vol. 40, E. Grushka (Ed.), Marcel Dekker (2000).
- 6. P.R. Brown, *Advances in Chromatography*, Vol. 37, E. Grushka (Ed.), Marcel Dekker (1997).
- 7. R.E. Ardrey, Liquid Chromatography Mass Spectrometry: An Introduction, John Wiley & Sons (2003).

Credit Hours: 03

Course Title: Chemistry of Isoprenoids and Steroids

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the two important classes of natural products i.e, isoprenoids and steroids. The knowledge can be applied in designing biologically important new compounds.

COURSE CONTENTS:

Introduction, classification, isolation, structure elucidation, reactions and biological activity: Terpenes, bile acids, cholesterol, ergosterol, vitamin D, estrogens, gastrogens, androgens, adrenocortical hormones, cardiac steroids and bufadienolides. **Total synthesis:** Equilinen, cholesterol, oestrone and epiandrosterone.

RECOMMENDED BOOKS:

- 1. D.F. Cane, D.H.R. Barton, K. Nakanishi and O. Meth-Cohn, *Comprehensive Natural Products Chemistry: Isoprenoids Including Carotenoids and Steroids*, Vol. 2, Elsevier Science Ltd. (1999).
- 2. K. Nakanishi, T. Goto, S. Ioto, S. Natori, S. Nozone, et al., *Natural Products Chemistry*, Vol. 1, Academic Press Inc, New York (1974).
- 3. F.L. Ansari, R. Quershi and M.L. Quershi, *Electrocyclic Reactions*, John Wiley & Sons (1999).

- 1. F.J. Leeper, Biosynthesis: Aromatic Polyketides, Isoprenoids, Alkaloids, Springer Verlag (2000).
- 2. S.V. Bhat, B.A. Nagasampagi and S. Minakshi, *Chemistry of Natural Products*, Narosa Publishing House (2005).
- 3. J.H. Fuhrhop and C. Endisch, *Molecular and Supramolecular Chemistry of Natural Products and Their Model Compounds*, Macel Dekker, Inc. New York (2000).

03

Credit Hours:

Course Title: Chemistry of Glycosides

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about glycosides that will enhance the skills in handling the naturally occurring compounds found as glycosides.

COURSE CONTENTS:

Introduction: Glycosides of flavonoids, coumarins and saponins, isolation, detection and chromatographic separation, biological importance of glycosides. **Chemical reactions:** Acid, alkaline and enzymatic hydrolysis to aglycones, derivatization. **Structure elucidation:** Identification of sugar residue, spectroscopic determination of aglyones and glycosides.

RECOMMENDED BOOKS:

- 1. R. Ikan (Ed.), Naturally Occurring Glycosides, Wiley, John & Sons, Inc. (1999).
- 2. B.A. Bohm, *Introduction to Flavonoids*, Harwood Academic Publishers, Canada (1998).
- 3. K.R. Markham, *Techniques of Flavonoid Identification*, Academic Press, London (1982).
- 4. J.B. Harborn, *The Flavonoids Advances in Research Since 1986*, Chapman & Hall, London (1994).

- 1. J. Mann, R.S. Davidson and J.B. Hobbs, *Natural Products: Their Chemistry and Biological Significance*, Longman Group UK Limited (1994).
- 2. D. Crich, Reagents for Glycoside, Nucleotide and Peptide Synthesis, John Wiley & Sons (2005).
- 3. D.E. Levy and C. Tang, *The Chemistry of C-glycosides*, Pergamon Press (1995).

- 4. K. Hostettmann and A. Marston, Saponins, Cambridge University Press (2005).
- 5. V. Ahmed and A. Basha, Spectroscopic Data of Saponins, Vol. III, CRC Press (2000).
- 6. R. O'Kennedy, R.D. Thornes, *Coumarins: Biology, Applications and Mode of Action*, John Wiley & Sons (1997).
- 7. R. Douglas, H. Murray and J. Méndez, *The Natural Coumarins: Occurrence, Chemistry, and Biochemistry*, Stewart Anglin Brown (1982).

Credit Hours: 03

Course Title:

Chemistry of Organometallic Compounds

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the organometallic compounds. The knowledge can be applied in designing synthesis of different catalysts.

COURSE CONTENTS:

Introduction, synthesis, reactivity and reactions: Grignard's reagents and alkyllithium. Applications: Alkyllithium as metallating agents in organic synthesis. Organotransition metal compounds: Organo palladium compounds, cupperates and organo zinc compounds, their synthesis and applications.

RECOMMENDED BOOKS:

- 1. M.Gielen, R. Willem and B. Warckmeyer (Eds.), *Physical Organometallic Chemistry*, Vol.3, John Willey and Sons, New York (2002).
- 2. L.S. Heqedus and L.G. Wade, *Transition Metals in the Synthesis of Complex Organic Molecules*, 2nd ed., John Willey and Sons. Ltd., New York (1999).
- 3. M. Schlosser, *Organometallics in Synthesis*, John Willey and Sons, Ltd. New York (1996).
- 4. A.W. Parking and R.C. Poller, *An Introduction to Organometallic Chemistry*, McMillian Education Ltd., New York (1987).
- 5. E.I. Negishi, *Organometallics in Organic Synthesis*, Vol.1, John Willey and Sons, New York (1980).

- 1. J. Clayden, N. Greeves, S. Warren and P. Worthers, *Organic Chemistry*, Oxford University (2001).
- 2. G.M. Loudon, *Organic Chemistry*, 4th ed., Oxford University Press, New York (2002).

03

Credit Hours:

Course Title: Organic Photochemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the organic photochemistry that will be helpful in synthesis of pericyclic compounds.

COURSE CONTENTS:

Introduction: Electronic structure of molecules, electronic transitions, radiative and non-radiative processes, energy transfer and sensitization, hydrogen abstraction. **Photochemical reactions:** Photo-elimination, photo-substitution, photo-oxidation and photo-reduction of carbonyl compounds and olefins. **Pericyclic reactions:** Photochemical dimerization, cycloadditions and rearrangements. **Applications:** Photochemical organic industrial processes.

RECOMMENDED BOOKS:

- 1. J.D. Coyle, *Introduction to Organic Photochemistry*, Wiley & Sons Inc. (1986).
- 2. J. Kopecky, Organic Photochemistry, John Wiley & Sons Inc. (1991).
- 3. A.G. Griesbeck, Synthetic Organic Photochemistry, Marcel Dekker Inc. (2004).
- 4. V. Ramamurthy, *Organic Photochemistry*, Marcel Dekker Inc. (1997).

- 1. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).
- 2. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, John Wiley & Sons (2007).

Credit Hours: 03

Course Title: Organic Polymer Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the organic polymer compounds important in designing of new synthetic materials.

COURSE CONTENTS:

Fundamental concepts: types of polymers, classification. Mechanism and kinetics: Step growth, free radical addition polymerization, ionic polymerization, Ziegler-Natta polymerization. Stereochemistry: Definition and examples of Isotactic, atactic, syndiotactic polymers and their stereoregulation. Molecular weight determination: Different methods used to determine the absolute and relative molecular weights of polymers. Structure-property relationship. Reactions of synthetic polymers. Polymer degradation and stability: Special emphasis on thermal and photodegradation.

RECOMMENDED BOOKS:

- 1. H.R. Allcock, F.W. Lampe and J.E. Mark, *Contemporary Polymer Chemistry*, 3rd ed., Pearson Education mc, Pearson Prentice Hall (2003).
- 2. F.W. Billrneyer Jr., *A Textbook of Polymer Science*, J. Wiley & Sons, Pte. Ltd., Singapore (1994).
- 3. G. Odian, Principles of Polymerization, 4th ed., John Wiley & Sons, Inc. (2004).

- 1. M.S. Bhatnagar, A Textbook of Polymers, Vol. I, II, III, S. Chand & Co. Ltd. (2004).
- 2. L.H. Sperling, *Introduction to Physical Polymer Science*, 2nd ed., John Wiley & Sons (1992).
- 3. J.R. Fried, *Polymer Science & Technology*, Prentice Hall, Inc. (1995).

Credit Hours: 03

Course Title: Pericyclic Reactions

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the pericyclic reactions and applying it the designing of new cyclic compounds.

COURSE CONTENTS:

Introduction and significance: Concerted and nonconcerted processes, pericyclic reactions, their classification and examples. **Mechanism and analysis:** Analysis of pericyclic reactions based on orbital symmetry conservation, frontier orbital method, Möbius-Hückel approach and theoretical & computational approach. **Synthetic application:** Synthesis of carbocycles and heterocycles through pericyclic reactions.

RECOMMENDED BOOKS:

- 1. F.L. Ansari, R. Qureshi and M.L. Qureshi, *Electrocyclic Reactions from Fundamentals to Research*, Wiley VCH (1999).
- 2. T.H. Lowry and K.H. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd ed., Harper & Row Publisher (1987).
- 3. F.A. Carey and R.J. Sandberg, *Advance Organic Chemistry*, Kulver Academic/Plenum Publisher (2000).

- 1. G.M. Loudon, *Organic Chemistry*, 3rd ed., The Benjamin/Cummings Publishing Company (1995).
- 2. E.A. Halevi, Orbital Symmetry and Reaction Mechanism, Springer Verlag (1992).
- 3. T. Rauk, *Orbital Interaction Theory of Organic Reaction*, John Wiley (1994).
- 4. R.T. Morrison and R.N. Boyd, *Organic* Chemistry, 6th ed., Prentice Hall, New Jersey (1992).

- 5. J. Clayden, N. Greeves, S. Warren and P. Worthers, *Organic Chemistry*, Oxford University (2001).
- 6. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).

Credit Hours: 03

Course Title: Cheminformatics

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about new field of cheminformatics that is useful in the overall understanding of organic compounds.

COURSE CONTENTS:

Basic concepts: Introduction, evolution, history and prospects. Database design & their management: Database concept and architecture, Structured Query Language (SQL), chemical database design & their tools, structure-based searches. Chemical information sources: History and future of scientific internet, chemical literature, communication in chemistry. Cheminformatics for drug discovery: Representation and manipulation of 2-D and 3-D molecular structures, computational models, similarity methods, analysis of high throughput screening data, virtual screening, combinatorial library designing, computing physical-chemical data and chemical registration systems.

RECOMMEND BOOKS:

- 1. A.R. Leach and V.J. Gillet, *An Introduction to Cheminformatics*, Kluwer Academic Publishers (2003).
- 2. R.B. Siverman, *The Organic Chemistry of Drug Design and Drug Action*, Academic Press (2004).
- 3. P.K. Larson, *A Textbook of Drug design and Development*, Overseas Publishers Associations OPA (1996).

SUPPLEMENTARY BOOK:

1. C.M. Bladen, Pharmaceutical Chemistry, John Wiley (2002).

Credit Hours:

03

Course Title: Advanced Stereoselective Synthesis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the stereoselective synthesis

useful in designing synthesis of complex compounds.

COURSE CONTENTS:

Biological significance of chirality: Stereogenic units and types of chirality, chiral natural

products, need for stereoselective synthesis. Strategies for synthesis of chiral

compounds: First and second generation methods: chiral starting materials and chiral

auxiliaries; third and fourth generation methods: asymmetric reactions, reagents and

catalysts. **Asymmetric total synthesis:** Diastereoselective and enantioselective syntheses.

RECOMMENDED BOOKS:

1. M. Nogradi, Stereoselective Synthesis: A Practical Approach Wiley VCH (1994).

2. R.S. Atkinson, Stereoselective Synthesis, Wiley, Chichester, (1995).

3. E.M. Carreira and O. Reiser, Classics in Stereoselective Synthesis, Wiley-VCH,

Weinheim (2007).

SUPPLEMENTARY BOOKS:

1. A. Koskinen, Asymmetric Synthesis of Natural Products, Wiley (1993).

2. Guo-Qiang Lin, Yue-Ming Li, Albert S. C. Chan, Principles and Applications of

Asymmetric Synthesis, Wiley-Interscience (2001).

3. G.R. Stephenson, Advanced Asymmetric Synthesis, Springer; 1st edition (1996).

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Credit Hours: 03

Course Title: Special Organic Materials

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the different organic materials.

COURSE CONTENTS:

Organic dyes: Chromophore structure, synthesis of azodyes and cyanins, reactive vs. direct textile dyes, Chemiluminescence, photochromocs, color photography. **Liquid Crystals:** definition, classification: thermotropic/lyotropic, calamitic/discotic, nematic/smectic columnar, synthesis and orientation, liquid crystal displays (LCD's), liquid crystal polymers. **Electronic materials:** Types of organic semi-conductors, polyacetylenes, and polyparaphenylenes, band structure, synthesis, electroluminescence and light emitting diodes (LED's).

RECOMMENDED BOOKS:

- 1. K.H. Klaus (Ed.), *Industrial Dyes*, Wiley-VCH, Verlag, GmbH & Co. (2003).
- 2. V.P. Shibaev and L. Lam (Eds.), *Liquid Crystalline and Mesomophoric Polymers*, Springer-Verlag, Inc., New York (1994).
- 3. P.J. Collings and M. Hird, *Introduction to Liquid Crystals: Chemistry and Physics*, Taylors and Francis (1997).

- 1. Dierking, Textures of Liquid Crystals, Wiley-VCH, Verlag, GmbH & Co. (2003).
- 2. J.W. Goodby and G.W. Gray, *Structures and Textures of Liquid Crystals*, Taylors and Frances (2006).
- 3. H. Zollinger, *Color Chemistry: Synthesis, Properties and Applications of Organic Dyes*, 3rd ed., Wiley-VCH (2003).
- 4. S.H. Kim (Ed.), Functional Dyes, Elsevier (2006).

5. T.S. Chung (Ed.), Thermotropic Liquid Crystal Polymers: Thin-Film Polymerization, Characterization, Blends and Applications (2001).

Credit Hours: 03

Course Title: Multicomponent Reactions

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the multicomponent reactions reactions and applying it to the designing of new versatile compounds with diverse applications.

COURSE CONTENTS:

General Introduction

Basic Concepts related with MCRs, Computational and Analytical Tools to Study MCRs, Diversity-Oriented Synthesis and Biology-Oriented Synthesis, Optimization of MCRs, Catalysis in MCRs and Various Synthetic Approaches, Importance and Evolution of MCRs

Organocatalytic Asymmetric Multicomponent Reactions

Three-Component Mannich Reaction, Cycloaddition Reaction, Organocatalytic Multicomponent Domino Asymmetric Reactions, Michael-Type Multicomponent Process

Metal-Catalyzed Multicomponent Reactions

Palladium-Catalyzed MCRs e.g, Carbonylation Reactions, Palladium-Catalyzed MCRs Involving Isocyanides, Carbopalladation of Unsaturated C-C π -Components, Amines as Building Blocks, Nickel-Catalyzed MCRs e.g, Cross-Trimerization of Alkynes, Reductive Conjugate Addition, Copper-Catalyzed Azide–Alkyne Cycloaddition, A3-Coupling, Rhodium-Catalyzed MCRs e.g, via Onium Ylide Intermediates and Cross-Addition Reactions, Ruthenium-Catalyzed MCRs

Multicomponent Reactions with Organoboron Compounds

Catalytic MCRs with Organoboron Compounds, Cobalt and Palladium-Catalyzed MCRs Containing Organoboron Compounds, Multicomponent Petasis-Borono–Mannich Reaction, Metal-Catalyzed Four-Component PBM Reaction, Multicomponent Hetero-Diels–Alder/Allylboration, Chiral ligands Catalyzed One-Pot [4 + 2] Cycloaddition/Allylboration, Polymer-Supported MCRs, Palladium-Catalyzed Asymmetric Allene Diboration/ α -Aminoallylation, Synthetic Applications of Boron-Based MCRs

Carbene-Promoted Multicomponent Reactions

MCRs Involving Carbenes as catalysts and ligands e.g, Dimethoxycarbenes, NHCs, FCCs, Approach to Highly Substituted Carbo- and Heterocycles

Multicomponent Reactions in the Synthesis of Target Molecules

MCRs in Drug Discovery and for the Synthesis of Biologically Important Molecules, Synthesis of Natural Products in an Efficient Manner, Heterocycles as Key Substrates like Indoles, Polyheterocycles, Spiro-Type Polyheterocycles, DHPMs and Thiazines, Pyrroles, Amino Acid Derivatives and other relevant Industrial Applications

Recent Advances in the Ugi Multicomponent Reactions

Ugi Three-, Four-, Five-, Six-, Seven-, and Eight-Component Reactions, Ugi Postmodification Processes, Ugi-Smiles Approach, Ugi-Smiles Postmodification Processes

Passerini Multicomponent Reactions

O-Alkylative, Arylative and Silylative Passerini Three-Component Reactions, Metal-Catalyzed O-Alkylative and O-Silylative Passerini Three-Component Reactions, Synthesis of Macrocycles by a Passerini Reaction, Enantioselective Metal-Catalyzed Passerini Reaction, Multicomponent Passerini Approach to Important Targets, α -Hydroxycarboxamide; an Important Intermediate for Chemical Synthesis, Passerini 3CR under Eco-Friendly Reaction Conditions, MW-Assisted Passerini Reaction

Biginelli Multicomponent Reactions

Mechanism, Chiral Lewis- and Brønsted Acid- and Base-Catalyzed One-Pot Three-Component Biginelli-Type Reactions, Organocatalytic Enantioselective Biginelli Reactions, Chiral Brønsted Acid-Organocatalyzed Biginelli Reactions, Aminocatalyzed Biginelli Reactions, Variations of the Traditional Biginelli Condensation

Bucherer-Bergs and Strecker Multicomponent Reactions

Bucherer–Bergs Reaction: Comparative Stereochemical Course, Synthesis of Five-Membered Heterocycles, Modified Bucherer–Bergs Reaction, Synthesis of α -Amino Acids via Hydantoin Intermediate, Synthesis of Diaminodicarboxylic Acids

Mc Strecker Reaction: Using Aldehyde, Strecker-Type Reaction Using Ketones, Catalyst-Free Strecker Reactions in Water, Catalyst-Free Strecker Reactions under Solvent-Free Conditions, Metal-Catalyzed Strecker-Type Reaction, Organocatalytic Mc Strecker Reaction, Efficient Heterogeneous Catalysis for the Synthesis of α -Aminonitriles, Synthetic Utility

Unusual Approach for Multicomponent Reactions

Zeolite-Catalyzed MCRs, Heterogeneous Hybrid Catalyst, MW-Assisted Three-Component Reactions, Synthesis of Natural Products, Ionic Liquid-Promoted MCRs, MCRs under Solvent-Free Conditions, MCRs in Aqueous Media, High-Pressure Promoted MCRs, Three-Component Reactions Using Supported Reagents

Some important Named Multicomponent Reactions

Radziszewski Reactions (Imidazole Synthesis), Sakurai MCRs: Synthesis of Homoallylic Ethers, Gewald MCRs: Easy Protocol for Synthesizing 2-Aminothiophene Derivatives, Kabachnik–Fields Reactions: Straightforward Synthesis of α -Amino Phosphonates, Knoevenagel Reactions in Multicomponent Syntheses: Domino Knoevenagel/Hetero-Diels–Alder Reaction and Pyran

Syntheses, Useful Syntheses of Heterocycles: 1,4-Dihydropyridine and Diazine Syntheses, Useful Syntheses of Heterocycles: Various Heterocyclic Scaffolds, Yonemitsu-Type Trimolecular Condensations: Introduction and Mechanistic Aspects, Applications of the Original Yonemitsu Trimolecular Condensation, Yonemitsu-Type Reactions and Tetramolecular Condensations, MCRs Involving Meldrum's Acid: Applications and DOS, Meldrum's Acid as Synthetic Equivalent, Meldrum's Acid as Malonic Acid Equivalent, Povarov MCRs: Efficient Synthesis of 1,2,3,4-Tetrahydroquinolines, Efficient Synthesis of Quinolines, Hantzsch Multicomponent Synthesis of Heterocycles: Catalysis and Mechanism, Syntheses of 1,4-Dihydropyridines and Their Oxidation to Pyridines, Multicomponent Pyrrole Syntheses

RECOMMENDED BOOKS:

- 1. R. P. Herrara, E. M. Lopez, Multicomponent reactions; concepts and applications for design and synthesis, Wiley (2015) ISBN: 978-1-118-86397-8
- 2. Thomas JJ. Muller, Multicomponent reactions, Thieme (2014) ISBN: 978-3131765611
- 3. E. V. Eycken, U. K. Sharma, *Multicomponent reactions towards heterocycles*, Wiley (2021) ISBN: 978-3-527-83244-6
- 4. J. Zhu, Hugues Bienaymé, *Multicomponent reactions*, Wiley (2006) ISBN: 978-3-527-60424-1

SUPPLEMENTARY BOOKS:

- 1. G.M. Loudon, *Organic Chemistry*, 3rd ed., The Benjamin/Cummings Publishing Company (1995).
- 2. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th ed., Prentice Hall, New Jersey (1992).
- 3. J. Clayden, N. Greeves, S. Warren and P. Worthers, *Organic Chemistry*, Oxford University (2011).
- 4. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).
- 5. F.A. Carey and R.J. Sandberg, *Advance Organic Chemistry*, Kulver Academic/ Plenum Publisher (2000).

Credit Hours: 03

Course Title: Transition Metal Catalyzed Organic Synthesis

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the multicomponent reactions reactions and applying it to the designing of new versatile compounds.

COURSE CONTENTS:

<u>Introduction:</u> The Basics, The Basic Structural Types, Just How Many Ligands Can Fit around a Metal Atom? Mechanism and the Basic Reaction Steps, Catalysis

<u>Coupling Reactions:</u> Carbon–Carbon Bond Formation, Lithium and Magnesium: Kumada Coupling, Zinc: The Negishi Reaction, Aluminium and Zirconium, Tin: The Stille Reaction, Boron: The Suzuki Reaction, Silicon: The Hiyama Reaction, Copper: The Sonogashira Reaction, Other Metals, Homocoupling, Enolate and Phenoxide Coupling, Heteroatom Coupling

<u>C-H Activation:</u> Arenes and Heteroarenes, Aldehydes, Borylation and Silylation, Allylic Functionalization, Unfunctionalized C-H Bonds

<u>Carbonylation:</u> Carbonylative Coupling Reactions: Synthesis of Carbonyl Derivatives, Carbonylative Coupling Reactions: Synthesis of Carboxylic Acid Derivatives, Carbonylation of Alkenes and Alkynes, Hydroformylation, Stoichiometric Carbonylation Using Carbonyl Complexes, Carboxylation, Decarbonylation and Decarboxylation

<u>Alkene and Alkyne Insertion Reactions:</u> The Heck Reaction, Insertion Reactions Involving Zirconium and Titanium

Electrophilic Alkene and Alkyne Complexes: Electrophilic Palladium Complexes, Other Metals: Silver, Gold, Platinum and Rare Earths, Iron Cobaloxime η-Cations

<u>Reactions of Alkyne Complexes:</u> Alkyne Cobalt Complexes, Propargyl Cations: The Nicholas Reaction, The Pauson–Khand Reaction, Synthesis Using Multiple Cobalt Reactions

<u>Carbene Complexes:</u> Fischer Carbenes, Vinylidene Complexes, Metathesis Reactions Involving Carbene Complexes, Carbyne Complexes, Carbene Complexes from Diazo Compounds

<u>n</u>³- or π-Allyl Complexes: Stoichiometric Reactions of π-Allyl Complexes, Catalysis: Mostly Palladium, Propargyl Compounds

<u>Diene, Dienyl and Arene Complexes:</u> $η^4$ -Diene Complexes, $η^5$ -Dienyl Complexes, $η^6$ -Arene Complexes

<u>Cycloaddition and Cycloisomerization Reactions:</u> Formal Six-Electron, Six-Atom Cycloadditions, Cycloadditions Involving Fewer than Six Atoms, Cycloadditions Involving More than Six Atoms, Isomerization, Cycloisomerization and Related Reactions

Formation of carbon-carbon bonds

Concepts for the Use of Transition Metals in Industrial Fine Chemical Synthesis, Hydroformylation, Amidocarbonylation of Aldehydes, Cyclopropanation, Isomerization of Olefin and the Related Reactions, Suzuki Reaction, Transition Metal-Catalyzed Arylation of Amines and Alcohols, Heck Reaction, Palladium-Catalyzed Allylic Substitutions Fischer-Type Carbene Complexes, Chromium-Arene Complexes

Reductions-oxidations

Homogeneous Hydrogenations, Heterogeneous Hydrogenations, Transferhydrogenations, Hydrosilylations, Oxidations of C-H Compounds Catalyzed by Metal Complexes, Metal-Catalyzed Baeyer-Villiger Reactions, Asymmetric Aminohydroxylation - Recent Developments, Rhenium-Catalyzed Epoxidations, Wacker-Type Oxidations, Two-Phase Catalysis Transition Metal Catalysis under High Pressure in Liquid Phase, Transition Metal Catalysis using Ionic Liquids

RECOMMENDED BOOKS:

- 1. Mathias Beller, Carsten Bolm, *Transition metals for Organic synthesis*, Wiley (2008). ISBN: 978-3-527-61940-5
- 2. Francois Diederich, Peter J. Stang, *Metal catalyzed cross coupling reactions*, Wiley (2009). ISBN: 978-3-527-61220-8
- 3. Armin de Meijere, Stefan Brase, Martin Oestereich *Transition Metals Organic synthesis*, Thieme (2013) ISBN: 978-3-527-65560-1

SUPPLEMENTARY BOOKS:

- 1. G.M. Loudon, *Organic Chemistry*, 3rd ed., The Benjamin/Cummings Publishing Company (1995).
- 2. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th ed., Prentice Hall, New Jersey (1992).
- 3. J. Clayden, N. Greeves, S. Warren and P. Worthers, *Organic Chemistry*, Oxford University (2011).
- 4. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).
- 5. F.A. Carey and R.J. Sandberg, *Advance Organic Chemistry*, Kulver Academic/ Plenum Publisher (2000).

PHYSICAL CHEMISTRY

Course Code: CH-861

Credit Hours: 03

Course Title: Physical Chemistry of High Polymers

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will obtain knowledge of various aspects of polymer such as molecular forces and bonding, geometry, morphology, analysis, properties and applications of polymers.

COURSE CONTENTS:

Introduction; Mechanisms of polymer synthesis; Molecular forces and chemical bonding in polymers; Configuration and conformation of polymer chains; Dimensions of polymer chains; Theories of Polymer solutions; Phase separation and fractionation; Criteria for polymer solutions; Solutility parameters; Thermodynamic studies of dilute and concentrated solutions of polymers; Plasticization; Molecular size measurements; Methods for measuring number-average weight average, z-average and viscosity average molecular weights; Applications of spectroscopic techniques (UV-Visible, IR and NMR) and Thermal analysis (TGA, DTA and glass transition) in polymer science; Electrical and magnetic properties of polymers; Industrial applications of polymers.

- 1. Billmeyer, F.W. Jr. 2005. Textbook of Polymer Science, John Wiley and Sons, New York, USA.
- 2. Crompton, T. R. 2009. Characterization of Polymers. Vol 1 & 2. Chem Tec Publishing, USA.
- 3. Francisco, J., B. Calleja and R. Zbigniew. 2000. Block copolymers, Marcel Dekker, Publishers, New York.
- 4. Joel, R.F. 2014. Polymer Science and Technology. 3rd Ed Prentice Hall Publishers, New York, USA.
- 5. Kurt, E.G. 2003. Advanced Macromolecular, Supramolecular Materials and Processes. Kluwer Academic/Plenum Publishers, New York, USA.
- **6.** Richards, R.W. and S.K. Peace. 1999. Polymer Surfaces and Interfaces, John Wiley and Sons, New York, USA.

Credit Hours: 03

Course Title: Advanced Surface Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will learn advanced concepts of surface science, interfaces and various aspects of adsorption phenomenon, colloidal dispersions and catalysis.

COURSE CONTENTS:

Adsorption, Mechanism of adsorption, Difference between adsorption and absorption, Types of adsorption, Physical adsorption, Chemical adsorption, Comparison of chemical and physical adsorptions, Characteristics of adsorption, Applications of adsorption, Factors affecting the process of adsorption, Adsorption isotherms, Freundlich adsorption isotherm, Derivation of the Freundlich adsorption equation, Postulates of Langmuir adsorption isotherm, Derivation of the Langmuir adsorption equation, Validity of Langmuir adsorption isotherm, Merits and demerits of Langmuir adsorption isotherm, Brunauer-Emmett-Teller (BET) adsorption isotherm, Postulates of BET adsorption isotherm, Derivation of the BET adsorption equation, Conversion of BET adsorption equation into straight line equation, Conversion of BET adsorption equation into Langmuir equation, Measurement of surface area of adsorbent using BET equation, Limitations of BET isotherm, Advantages of BET isotherm, BET isotherm versus Langmuir adsorption isotherm, Dubinin-Raduschkevich adsorption isotherm, Application of the Langmuir, Freundlich and D-R models to the adsorption isotherm data in Microsoft excel, Mechanism of adsorption kinetics, Applications of pseudo first and pseudo second order models to the adsorption kinetic data in Microsoft excel, Adsorption with dissociation, Competitive adsorption.

Suggested Readings:

- Adamson, A.W. 1997. Physical Chemistry of Surfaces. 6th Ed. John Wiley and Sons, New York, USA.
- 2. Hiemenzt, and M.C. Rajagopalan. 1997. Principles of Colloid & Surface Chemistry, 3rd Ed., P.C., McGraw-Hill New York.
- 3. Birdi, K.S. 2013.Handbook of Surface and Colloidal Chemistry, CRC Press, New York, USA
- 4. Bubert, H. and H. Jenett. 2011. Surface and Thin Film Analysis: Principles, Instrumentation, Applications, Wiley-VCH, Verlag GmbH, Germany.

5. Somorjai, G. A., and L. Yimin. 2010. Introduction to Surface Chemistry and Catalysis. John Wiley & Sons. New York, USA.

Credit Hours: 03

Course Title: Advanced Solution Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students would get knowledge about various aspects of solution chemistry and would be able to apply them in industry.

COURSE CONTENTS:

Solutions: Classification; their importance in chemistry, industry and life science. Interactions in solutions: Concept of solute and solvent; multicomponent systems; preferential solvation. Solvents: Their characterization; microscopic structure of solvent and solvates; pair distribution function (PDF) and its determination using different techniques (spectroscopy and diffraction). Molecular dynamics and microscopic structure; different techniques of molecular dynamical calculations. Theories and laws related to solutions. Macroscopic properties of solutions: Transport properties; thermodynamics of solution; equilibria in solutions.

- 1. Reichhardt, C. 1988. Solvents and Solvent Effects in Organic Chemistry. 2nd Ed., VCH, Weinheim, Germany.
- 2. Hildebrand, J. H., J.M. Prausnitz and R.L. Scott. 1970. Regular and Related Solutions. Van Nostrand Reinhold Company, New York.
- Popovych, O. and R.P.T. Tomkins. 1981. Nanoaqueous Solution Chemistry. John Wiley & Sons, New York. 4. Tabor, D. 1993. Gases, Liquids and Solids. 3rd Ed., Cambridge University Press, UK.
- 4. Reid, R. C. and T.K. Sherwood. 1986. The Properties of Gases and Liquids. McGraw-Hill Book Company, New York.
- 5. Shinoda, K. 1988. Principles of Solution and Solubility. Marcel Dekker, Inc., New York.

Credit Hours: 03

Course Title: Tribology

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students would get knowledge about advanced composite materials, their mechanical, dynamical (Tribological) and thermal properties.

COURSE CONTENTS:

Definitions and Classification; Property enhancement by reinforcement and orientation, Matrix interface, Synthetic fibres; Properties and processing of composites with metallic, ceramic and polymeric matrices; Carbon based composite materials; Interface reactions; Mechanical and thermal properties of composite materials; Dynamical mechanical properties; Toughening mechanisms and mechanical failure in polymeric composites.

- 1. Carlsson, L.A., D.F. AdamsandR.B. Pipes. 2014. Experimental Characterization of Advanced Composite Materials. CRC Press, London, UK.
- 2. Nicolais, L., M. Meo and E. Milella. 2011. Composite Materials: A Vision for the Future. Springer-Verlag, London, UK.
- 3. Carlsson, L.A., D.F. AdamsandR.B. Pipes. 2014. Experimental Characterization of Advanced Composite Materials. CRC Press, London, UK.
- 4. Carlsson, L.A., D.F. AdamsandR.B. Pipes. 2014. Experimental Characterization of Advanced Composite Materials. CRC Press, London, UK.

Credit Hours: 03

Course Title: Recent Advances in Physical Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will obtain knowledge related to some of the current advancements in Physical Chemistry.

COURSE CONTENTS:

Latest advances in physical chemistry in: Solution chemistry; Energy materials; Green and sustainable chemistry; Lasers chemistry; Femto techniques in chemistry; Advanced materials for waste water treatment; Supramolecular chemistry; Modern software used in chemistry. Analytical review of latest books and research papers/review articles.

- 1. Atkins, P. and J. de Paula. 2011. Elements of Physical Chemistry. 7th Ed. W.H. Freeman and Company, New York, USA.
- 2. Helmet H.T, A. G. Urena and R. J. Donovan. 2007. Laser Chemistry: Spectroscopy, Dynamics and Application. John Wiley and Sons, New York, USA.
- 3. Marcus, Y. 1999. The Properties of Solvents. John Wiley and Sons, New York, USA.
- 4. MihkelKoel, 2009, Ionic Liquids in Chemical Analysis. CRC Press Taylor & Francis, New York, USA.
- 5. Monique, M. Martin, James T. Hynes, 2004, Femtochemistry and Femtobiology Ultrafast Events in Molecular Science, Elsevier Ltd. London, UK.
- 6. Rolando, M.A., and M. Roque-Malherbe. 2009. The Physical Chemistry of Materials: Energy and Environmental Applications. CRC Press Taylor & Francis, New York, USA.

Credit Hours:

03

Course Title: Advanced Statistical Mechanics

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will obtain knowledge related to some of the current advancements in statistical

mechanics and their applications.

COURSE CONTENTS:

Introduction: Statistical mechanics and its significance for chemical systems. Ensembles:

microcanonical, canonical and grand canonical. Probability: Discrete states; continuously

varying probabilities. Average values: concepts of number average and time average,

fluctuations and standard deviations. Partition functions: Concept; different types; their

determination for diatomic and polyatomic molecules. Partition functions of the systems of

very large number of particles. Relationship between partition function and thermodynamic

functions. Statistical mechanical treatment: Chemical equilibria and chemical reactions;

imperfect gases; liquid state; dilute solutions: perfect crystals. Applications of Ferm-Dirac

and Bose-Einstein statistics and their mutual comparison with Boltzman Maxwell

statistics.

RECOMMENDED BOOKS:

1. F. Reif, Statistical Physics (Berkeley Physics Course), McGraw-Hill, New York (1965).

2. N. Davidson, Statistical Mechanics, McGraw-Hill, New York (1962).

3. T.L. Hill, Statistical Mechanics, McGraw-Hill, New York (1956).

4. J.G. Aston and J.J. Fritz, Thermodynamics and Statistical Thermodynamics, John-

Wiley, New York (1959).

5. J.M. Seddon and J.D. Gale, Thermodynamics and Statistical Mechanics, RSC

Publishers (2001).

Credit Hours: 03

Course Title: Applied Chemical Thermodynamics

COURSE LEARNING OBJECTIVES AND OUTCOMES:

The students will be able to obtain knowledge about the application of chemical thermodynamics, phase equilibrium and gas and liquid mixtures.

COURSE CONTENTS:

Basic thermodynamics: Energy balance; entropy balance. Thermodynamic properties interrelations: Maxwell's equations; flow of fluids. Power production: The Rankine cycle, Brayton's cycle; fuel cells and batteries; internal combustion engine; compression and refrigeration. Vapor compression evaporation; vapor compression refrigeration, liquefaction of gases. Phase equilibrium: Non-ideal gas and liquid mixtures; chemical reaction equilibria.

RECOMMENDED BOOKS:

- 1. J. Winnik, *Chemical Engineering Thermodynamics*, John Wiley & Sons, Inc., New York (1997).
- 2. I.N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).

SUPPLEMENTARY BOOKS:

- 1. B.G. Kyle, *Chemical and Process Thermodynamics*, Printice Hall International, London (1999).
- 2. T. Letcher (Ed.), *Chemical Thermodynamic for Industry*, Royal Society of Chemistry, ISBN: 0854045910 (2004).

03

Credit Hours:

Course Title: Theoretical and Computational Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

The students will be able to learn about the fundamentals of theoretical and computational chemistry and its applications in applied research.

COURSE CONTENTS:

Introduction to computational chemistry: Basic concepts of quantum mechanics, history of development of computational chemistry and its applications, relevance of hardware and software components. Molecular mechanics: Force field energies and parametrization, geometry optimization and molecular modeling, potential energy surfaces. Molecular orbital calculations: Solution of the Schrodinger wave equation for molecular orbitals, Huckel molecular orbital theory and self consistent Hartree Fock method. Semiempirical and ab-initio molecular orbital calculations. Hybrid quantum mechanical and molecular mechanical methods. Correlation of experimental and theoretical results: Quantitative significance and interpretation of theoretical results. Relationship of theoretical results with spectral and molecular properties. Relationship of theoretical results to chemical reactivity indices. Interpretation and prediction of reaction mechanism using reactivity indices. Density functional theory (DFT): Philosophy, early applications, Hohenberg-Kohn variational theorem. Advantages of DFT compared to MO theory.

RECOMMENDED BOOKS:

- 1. C.J. Cramer, Essentials of Computational Chemistry, John Wiley and Sons (2002).
- 2. F. Jenson, Introduction to Computational Chemistry, Wiley, Chichester (2000).

SUPPLEMENTARY BOOK:

1. K.B. Lipkowitz and D.B. Boyd, *Reviews in Computational Chemistry*, VCH, New York (1991).

Credit Hours: 03

Course Title: Chemistry of Advance Materials

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students would get knowledge about the chemistry of advanced materials, their structure, kinetics and processing.

COURSE CONTENTS:

Solubility limit: Phases; microstructure; phase equilibria; interpretation of phase diagrams. **Isomophous alloys:** Binary eutectic systems. Congruent phase transformation. Gibbs phase rule. Kinetics of phase transformation; multiphase transformation. **Structure of materials:** Metals; alloys; ceramics; gases; polymers; composite and biologic. Thermodynamics of condensed phases. **Kinetic processes in materials:** momentum, heat, and mass transport properties of materials. Mechanical, electrical, magnetic and optical properties of materials. **Processing of materials.** Case studies in material's selection.

RECOMMENDED BOOKS:

- 1. W.D. Callister, Jr., *Material Science and Engineering*, 6th ed., John Wiley, New York (2003).
- 2. M. Schwartz, New Materials, Process, and Methods Technology, CRC Press, New York (2006).

SUPPLEMENTARY BOOK:

1. B.S. Mitchell, *An Introduction to Materials Engineering and Science for Chemical and Materials Engineers*, John Wiley, New York (2003).

Credit Hours: 03

Course Title: Advanced Techniques in Physical Chemistry

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students would get knowledge about advanced techniques use in Physical chemistry for understanding various aspects in the field.

COURSE CONTENTS:

Magnetic resonance spectroscopy: Introduction, different types of magnetic resonance imaging (MRI), measurement of proton density, measurement of cerebral blood flow, measurement of cerebral blood volume, measurement of fractional anisotropy, nuclear magnetic resonance (NMR) in solid state, measurement of scalar couplings, measurement of dipolar couplings, measurement of "residual dipolar couplings". Diffraction methods: Introduction, single crystal X-ray diffraction (XRD) of small molecules and macromolecules including natural systems; powder X-ray diffraction (XRD) of small molecules and macromolecules, measurement of lattice parameters, measurement of B-values, determination of space group, calculation of electron density map. Electron microscopy: Introduction, scanning electron microscopy (SEM), transmission electron microscopy (TEM), measurement of I/Q values, single particle 3-D reconstruction. Fluorescence techniques: Steady-state fluorescence, time-resolved fluorescence, measurement of fluorescence anisotropy.

- 1. E.M. Haacke, R.W. Brown, M.L. Thompson and R. Venkatesan, *Magnetic Resonance Imaging: Physical Principles and Sequence Design*, John Wiley, New York (1999).
- 2. M.J. Duer, *Introduction to Solid-State NMR Spectroscopy*, Blackwell Publishing (2004).
- 3. J.P. Glusker, M. Lewis and M. Rossi, *Crystal Structure Analysis for Chemists and Biologists*, VCH Publishers, New York (1994).
- 4. J. Kuo, *Electron Spectroscopy: Methods and Protocols*, Humana Press (2007).
- 5. A. Sharma and S.G. Schulman, *Introduction to Fluorescence Spectroscopy*, Wiley Interscience (1999).

Credit Hours: 03

Course Title:

Research Methodology

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students would get knowledge about methods and techniques used in research. The students will learn about how to prepare research proposal, case study, thesis and research articles.

COURSE CONTENTS:

Importance of research in higher education, identification of a research topic; formulation of research questions; undertaking a literature study; collection and analysis of relevant data and developing a written sustained argument linking theory and evidence. Role of computers in research; writing research proposals; research methods for chemical sciences. Plagiarism; why and where to publish; research ethics. Scientific report writing; editing and proof reading of research work; data collection and data analysis; research design, analyzing abstracts and data collection tool; using online resources for research; sharing and discussing case studies; documentation of research.

DISSERTATION/RESEARCH/SEMINAR

Course Code: CH-890

Credit Hours: 12

Course Title: Research

The student has to conduct research on specific topic under supervision of faculty member.

Thesis

The student shall submit a thesis on the subject of his/her research work for evaluation and an oral examination.

Seminar on Research / Thesis

The student shall give a seminar on the topic of his/her research.