Description of Courses

for

M.Phil & PhD

Institute of Chemical Sciences

University of Swat

RECOMMENDED BY BOARD OF STUDIES IN ITS MEETING HELD ON JULY 03, 2018
FOR APPROVAL FROM UNIVERSITY STATUTORY BODIES

Table of Contents

Introduction

The description of courses for MPhil and PhD was presented before the board of studies in its meeting scheduled on July 03, 2018 for recommendations and approval.

The board of studies includes following worthy members

1. Dr. Ihsan Ullah, Institute of Chemical Sciences, university of Swat. (Convener)
2. Prof. Dr. Imtiaz Ahmad, ICS, University of Peshawar. (Expert Member)
3. Prof. Dr. Mumtaz Ahmad, Deptt: of Chemistry, GPGJC, Swat. (Expert Member)
4. Prof. Dr. Manzoor Ahmad, Deptt: of Chemistry, University of Malakand. (Expert Member)
5. Dr. Ahmad Ali, Centre for Plant Sciences and Biodiversity, University of Swat. (Member)
6. Dr. Ghaus Ur Rahman, Deptt: of Mathematics and Statistics, University of Swat. (Member)
7. Mr. Babar Azam, Department of Physics, GPGJC, Swat. (Member)
8. Mr. Nasib Rawan, Department of Chemistry, GDC, Mingora, Swat. (Member)
9. Dr. Zakir Ullah, Department of Physics, University of Malakand. (Member)
10. Dr. Adnan, Institute of Chemical Sciences, University of Swat. (Member /Secretary)

Mission Statement

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 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. We envision our institute to play a leading role in teaching and research and expect our graduates will serve the nation and humanity.

Objectives:

- To impart knowledge and training to students of MPhil and PhD in the field of Chemistry 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

Semester-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
Semester-II				
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
Semester-III & IV				
9	Research / Thesis / Seminar	CH-790	6 (0-6)	200
		Total	30 (24-6)	1000

* 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

Analytical Chemistry

Course Code	Course Title	Credit Hours
CH-701	Separation Techniques	3-0
CH-702	Analysis and Characterization of Polymers	3-0
CH-703	Atomic Spectroscopy	3-0
CH-704	Chromatographic Methods of Analysis	3-0
CH-705	Composite Materials	3-0

Inorganic Chemistry

Course Code	Course Title	Credit Hours
CH-721	Medicinal Inorganic Chemistry	3-0
CH-722	Inorganic Electronic Spectroscopy	3-0
CH-723	Kinetics and Mechanisms of Inorganic Reactions	3-0
CH-724	Physical Methods in Inorganic Chemistry	3-0
CH-725	Inorganic Material Chemistry	3-0
CH-726	Special Topics in Inorganic Chemistry	3-0

Organic Chemistry

Course Code	Course Title	Credit Hours
CH-741	Organic Synthesis-Retrosynthetic Approach	3-0
CH-742	Advanced Stereochemistry	3-0
CH-743	Nuclear Magnetic Resonance in Organic Chemistry	3-0
CH-744	Biosynthesis of Natural Products	3-0
CH-745	Reactive Intermediates in Organic Chemistry	3-0
CH-746	Advanced Heterocyclic Chemistry	3-0
CH-747	Advanced Mass Spectrometry	3-0
CH-748	Special Topics in Organic Chemistry	3-0
CH-749	Medicinal Chemistry	3-0

Physical Chemistry

Course Code	Course Title	Credit Hours
CH-761	Advanced Chemical Kinetics	3-0
CH-762	Chemical and Statistical Thermodynamics	3-0
CH-763	Quantum Chemistry	3-0
CH-764	Molecular Spectroscopy	3-0
CH-765	Environmental Chemistry	3-0
CH-766	Colloid Chemistry	3-0
CH-767	Polymer Chemistry	3-0
CH-768	Heterogeneous Catalysis	3-0

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

Semester-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
Semester-II				
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
Semester-III & IV				
7	Research / Thesis / Seminar	CH-890	12 (0-12)	400
		Total	30 (18-12	1000

* 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

Analytical Chemistry

Course Code	Course Title	Credit Hours
CH-801	Nano Chemistry	3-0
CH-802	Nuclear Methods of Analysis	3-0
CH-803	Advanced Chromatographic Techniques	3-0
CH-804	Molecular Spectroscopy	3-0
CH-805	Advanced Analytical Instrumental Techniques	3-0
CH-806	Advanced Thermal Analysis	3-0

Inorganic Chemistry

Course Code	Course Title	Credit Hours
CH-821	Advanced Nuclear and Radiation Chemistry	3-0
CH-822	Organo-transition Metal Chemistry	3-0
CH-823	Bio-Inorganic Chemistry	3-0
CH-824	Catalysis	3-0

Organic Chemistry

Course Code	Course Title	Credit Hours
CH-841	Modern Name Reactions in Organic Synthesis	3-0
CH-842	Computational Chemistry/Molecular Modeling	3-0
CH-843	Protecting Groups in Organic Synthesis	3-0
CH-844	Physical Organic Chemistry	3-0
CH-845	Advances in Chromatographic Techniques	3-0
CH-846	Chemistry of Isoprenoids and Steroids	3-0
CH-847	Chemistry of Glycosides	3-0
CH-848	Chemistry of Organometallic Compounds	3-0
CH-849	Organic Photochemistry	3-0
CH-850	Organic Polymer Chemistry	3-0
CH-851	Pericyclic Reactions	3-0
CH-852	Cheminformatics	3-0
CH-853	Advanced Stereoselective Synthesis	3-0
CH-854	Special Organic Materials	3-0

Physical Chemistry

Course Code	Course Title	Credit Hours
CH-861	Physical Chemistry of High Polymers	3-0
CH-862	Advanced Surface Chemistry	3-0
CH-863	Advanced Solution Chemistry	3-0
CH-864	Tribology	3-0
CH-865	Recent Advances in Physical Chemistry	3-0
CH-866	Advanced Statistical Mechanics	3-0
CH-867	Applied Chemical Thermodynamics	3-0
CH-868	Theoretical and Computational Chemistry	3-0
CH-869	Chemistry of Advance Materials	3-0
CH-870	Advanced Techniques in Physical Chemistry	3-0

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 Chromatography (FPLC): Principle and work flow, Cation/ Anion exchange chromatography, hydrophobic interaction Chromatography. Optimization of conditions and calibration of Instrumentation. Ion Exchange Chromatography, gel filtration 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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-702**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-703**

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.

RECOMMENDED BOOKS

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.

Course Code: **CH-704**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-705**

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.

RECOMMENDED BOOKS:

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).

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-722**

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).

Course Code: **CH-723**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-724**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-725**

Credit Hours: **03**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-726**

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).

Course Code: **CH-742**

Credit Hours: **03**

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).

Course Code: **CH-743**

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).

Course Code: **CH-744**

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).

Course Code: **CH-745**

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).

Course Code: **CH-746**

Credit Hours: **03**

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).

Course Code: **CH-747**

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).

Course Code: **CH-748**

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).

Course Code: **CH-749**

Credit Hours: **03**

Course Title: **Medicinal Chemistry**

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

2 **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,

RECOMMENDED BOOKS:

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.

Course Code: **CH-762**

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.

RECOMMENDED BOOKS:

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

Course Code: **CH-763**

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.

RECOMMENDED BOOKS:

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

Course Code: **CH-764**

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

RECOMMENDED BOOKS:

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

Course Code: **CH-765**

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.

2 **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,

3 **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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-766**

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.

RECOMMENDED BOOKS:

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

Course Code: **CH-767**

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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-768**

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.

4. **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.

RECOMMENDED BOOKS:

1. 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. Nanoscale, Nanometer, Nanoparticles, Nanotubes, Thin films, 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)

Course Code: **CH-802**

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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-803**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-804**

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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-805**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-806**

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.

RECOMMENDED BOOKS:

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).

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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-822**

Credit Hours: **03**

Course Title: **Organo-transition Metal Chemistry**

COURSE LEARNING OBJECTIVES AND OUTCOMES:

Students will acquire knowledge and understanding about the chemistry of organo-transition 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 η2−η7. 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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-823**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-824**

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.

RECOMMENDED BOOKS:

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:

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).

Course Code: **CH-842**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-843**

Credit Hours: **03**

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).

Course Code: **CH-844**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-845**

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).

Course Code: **CH-846**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-847**

Credit Hours: **03**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-848**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-849**

Credit Hours: **03**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-850**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-851**

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).

SUPPLEMENTARY BOOKS:

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).

Course Code: **CH-852**

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).

Course Code: **CH-853**

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).

Course Code: **CH-854**

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).

SUPPLEMENTARY BOOKS:

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).

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 solubility; Solubility 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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-862**

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:

1. 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.

Course Code: **CH-863**

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.

RECOMMENDED BOOKS:

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.
3. 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.

Course Code: **CH-864**

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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-865**

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.

RECOMMENDED BOOKS:

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.

Course Code: **CH-866**

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).

Course Code: **CH-867**

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).

Course Code: **CH-868**

Credit Hours: **03**

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).

Course Code: **CH-869**

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).

Course Code: **CH-870**

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.

RECOMMENDED BOOKS:

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).

Course Code: **CH-**

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.

Course Code: **CH-**

Credit Hours: **03**

Course Title: **Review Paper/Position Paper**

A thorough literature review related to research project/current topic of interest be carried out and to submit the assigned report at the end of the semester. The written report should take the form of a review article written for an established scientific journal. The report should include the importance of the topic. Give a concise account of the ideas that underpin the topic of early studies in the area. Identify the major questions that surround the field of study and show how they emerge. Give an account of recent advances in the field and how these were achieved. Give experimental detail

where appropriate, especially when new techniques have been developed to answer specific problems. Use the relevant bibliography.

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.