CURRICULUM OF CHEMISTRY

BS Program (4-Year, 8-Semester)



Department of Chemistry

Shaheed Benazir Bhutto Women University Peshawar

SCHEME OF STUDIES

(Session 2016 onward)

Scheme	of	Studies
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Course Code	Course Title	Credit Hours
Semester – I		
EN-101	Functional English-I	3
PS-101	Introduction to Pakistan Studies	2
PH-101	Introductory Mechanics and Waves	2 + 1
MA-100 or	Basic Mathematics or	3
MA-101	Calculus and Analytical Geometry-I	3
CS-101	Introduction to Computing	3
CH-101	Chemistry-I	3 + 1
	Total:	18
MA-100/MA-101 at F.Sc. level.	will be offered to those students who have not studied Math	nematics/Chemistry
Semester – II		
EN-102	Functional English-II	3
IS-101	Islamic Studies/Ethics	2
PH-103	Electricity, Magnetism and Thermal Physics	2 + 1
MA-101 or	Mathematics-I or	3
MA-102	Mathematics-II	3
CS-102	Introduction to Programming	3
CH-102	Chemistry-II	3 + 1
	Total:	18
	ematics-I) will be offered only for those students who ha Aathematics) in 1 st semester	ve already passed
Semester – II		
ST-201	Applied Statistics	3
EN-201	English-III (Report Writing)	3
EC-201	Economics	3
CH-201	Chemistry-III	3+1
CH-201 CH-202	Environmental Chemistry	4
011-202	Total:	17
Semester – IV		-
BY-201	Introductory Biology	3
GEN-400	Elective Social Sciences-I	3
CH-203	Chemistry-IV	3+1
CH-204	Industrial Chemistry	4
ES-202	Geo-tectonics	3
<u> </u>	Total:	17

Semester – V		
CH-301	Analytical Chemistry-I	3 + 1
CH-302	Inorganic Chemistry-I	3 + 1
CH-303	Organic Chemistry-I	3 + 1
CH-304	Physical Chemistry-I	3 + 1
	Total:	16
Semester – V	I	
CH-311	Analytical Chemistry-II	3 + 1
CH-312	Inorganic Chemistry-II	3 + 1
CH-313	Organic Chemistry-II	3 + 1
CH-314	Physical Chemistry-II	3 + 1
	Total:	16

Specialization (Inorganic-Analytical/Organic/Physical Chemistry)

Semester – V	II & VIII	
CH-401	Molecular Spectroscopy	3
CH-402	Atomic Spectroscopy	3
CH-403	Organometallic Chemistry	3
CH-404	Crystallography	3
CH-405	Inorganic Polymers	3
CH-406	Group Theory in Chemistry	3
CH-407	Chemical Process Industries	3
CH-408	Nuclear Methods of Analysis	3
CH-409	Coordination Chemistry	3
CH-410	Nano-Materials in Chemistry	3
CH-491	Inorganic/Analytical Chemistry Laboratory-III	3
Or	Or	
CH-497	Thesis/Research Project in Inorganic/Analytical Chemistry	
CH-494	Advanced Inorganic/Analytical Chemistry Laboratory	3
Or	Or	
CH-500	Thesis/Research Project in Inorganic/Analytical Chemistry	
	Total:	36

Inorganic/Analytical Chemistry

Note:- Five courses containing 15 credits will be offered in each semester.

Organic Chemistry

Semester – V	II & VIII		
CH-421	Chemistry of Heterocycles		3
CH-422	Reaction Mechanism-I		3
CH-423	Spectroscopic Methods in Organic Chemistry-I		3
CH-424	Chemistry of Natural Products		3
CH-425	Biochemistry		3
CH-426	Name Reactions		3
CH-427	Organic Polymer Chemistry		3
CH-428	Reaction Mechanism-II		3
CH-429	Stereochemistry		3
CH-430	Retrosynthesis		3
CH-431	Quantum Organic Chemistry		3
CH-432	Spectroscopic Methods in Organic Chemistry-II		3
CH-492	Organic Chemistry Laboratory-III		3
Or	Or		
CH-498	Thesis/Research Project in Organic Chemistry		
CH-495	Advanced Organic Chemistry Laboratory		3
Or	Or		
CH-501	Thesis/Research Project in Organic Chemistry		
	Τ	Total:	42

Note:- Five courses containing 15 credits will be offered in each semester.

Physical Chemistry

Semester – VII & VIII		
CH-441	Polymer Chemistry	3
CH-442	Molecular Spectroscopy	3
CH-443	Chemical Kinetics	3
CH-444	Solid State Chemistry	3
CH-445	Electrochemistry	3
CH-446	Nuclear and Radiation Chemistry	3
CH-447	Surface Chemistry	3
CH-448	Photochemistry	3
CH-449	Thermodynamics	3
CH-450	Solution Chemistry	3
CH-451	Colloids and Surfactants	3
CH-452	Quantum Chemistry	3
CH-453	Numerical Methods and Computational Chemistry	3
CH-454	Statistical Mechanics	3
CH-493	Physical Chemistry Laboratory-III	3
Or	Or	
CH-499	Thesis/Research Project in Physical Chemistry	
CH-496	Advanced Physical Chemistry Laboratory	3
Or	Or	
CH-502	Thesis/Research Project in Physical Chemistry	
	Total:	48

Note:- Five courses containing 15 credits will be offered in each semester.

Details of Theory/Practical Courses for BS (4-Years) Chemistry

BS 1st Year (Semester-I)

CH-101 Chemistry-I (Cr. 3)

The Periodic Law and Periodicity: Development of Periodic Table; Classification of elements based on *s*, *p*, *d* and *f* orbitals, group trends and periodic properties in *s*, *p*, *d* and *f* block elements, i.e., atomic radii, ionic radii, ionization potential, electron affinities, electronagetivities and redox potential.

Principles of Chemical Bonding: Types of chemical bonding; Lewis structures and prediction of shapes using VSEPR model, the localized bond approach: VB theory, hybridization and resonance; the delocalized approach to bonding: molecular orbital theory as applied to diatomic and polyatomic molecules, three center bonds, bonding theory of metals and intermetallic compounds; conductors, insulators and semiconductors; bonding in electron deficient compounds; hydrogen bonding.

Acids and Bases: Concepts of acids and bases including SHAB concept, relative strength of acids and bases, significance of pH, pKa, pKb and buffer solutions. Theory of indicators, solubility, solubility product, common ion effect and their industrial applications.

Chemistry of p-block Elements:Chemistry and structure of *p*-block elements; main emphasis on the chemistry and structure of noble gases and their compounds, chemistry and structure of interhalogens, pseudohalogens and polyhalides.

Recommended Books

- 1. Cotton, F. A., Wilkinson, G. and Gaus, P. L., "*Basic Inorganic Chemistry*", 3rd Ed., Wiley, New York, 1995.
- 2. Huheey, J. E., Keiter, E. A. and Keiter, R. L., "Inorganic Chemistry: Principles of Structure and Reactivity", 4th Ed., Harper and Row, New York, 2001.
- 3. Clyde Day, M. & Selbin, J., "*Theoretical Inorganic Chemistry*", 2nd Ed., Van Nustrand Reinhold, 1969.
- 4. Lee, J.D., "*Concise Inorganic Chemistry*", Chapman and Hall, 5th Ed., 1996.
- 5. Shriver, D. F., Atkins, P. W. and Langford, C. H., "Inorganic Chemistry", OxfordUniversity Press, 2nd Ed., 1994.
- 6. Bassette, J., Denney, G. H. and Mendham, J., "Vogel's Textbook of Quantitative Inorganic Analysis Including Elementary Instrumental Analysis" English Language Book Society, 4th Ed., 1981.

CH-101 Chemistry-I Lab. (Cr. 1)

- 1. Laboratory Ethics and Safety Measures: Awareness about the toxic nature of chemicals and their handling, cleaning of glassware, safe laboratory operations.
- 2. Qualitative Analysis: Analysis of four ions (two anions and two cations) from mixture of salts.

3. Quantitative Analysis:

- i) Volumetric Analysis: Practical exercises will be based on Redox, Iodometric and Iodimetric, Precipitation and Complexometric Reactions.
- ii) Gravimetric Analysis: Estimation of Ni^{2+} , Ba^{2+} . Determine percent of P and P_2O_5 in a sample of ammonium phosphomolybdate.

Recommended Book

1. Vogel, A. I., "A Textbook of Micro and Semi-micro Qualitative Inorganic Analysis" Longman Green & Co., 1995.

BS 1st Year (Semester-II)

CH-102 Chemistry-II (Cr. 3)

Physical Properties of Matter: Concept of ideal and real gases, state variables, equations of states (ideal gas equation and van der Walls equation). Kinetic model of gases; Collision diameter, mean free path, collision frequency. Properties of liquids; Surface tension, viscosity, refractive index, polarity, homogeneous and heterogeneous solutions, types of interactions in liquids, van der Waals interactions, dipole-dipole interactions, hydrogen bonding. Unit cell, crystal lattice, crystal systems, Miller indices, amorphous and crystalline solids. Thermodynamics: Thermodynamic system, surrounding, zeroth law of thermodynamics, concept of equilibrium, first law of thermodynamics, concept of internal energy, enthalpy, thermodynamic processes under different conditions (isothermal, adiabatic, reversibility concept), second law of thermodynamics, concept of entropy, Gibb's free energy. Chemical Kinetics: Rate of reactions, order of reactions, molecularity, extent of reaction, rate laws of zero-order and first-order reactions and differential and integrated forms, examples, concept of half-life and mean-life, factors affecting rates (Arrhenius equation). Electrochemistry: Introduction of electrochemistry (ions in solution, conductance, resistance); Ohm's law, Kohlrausch law, electrode potential, electrochemical cell (galvanic cell, electrolytic cell).

Pre-requisite: CH-101

Recommended Books

- 1. P.W. Atkins, and J. de Paula. *Physical Chemistry*, 8th ed., Freeman & Co., New York (2006).
- 2. R.A. Alberty and R.J. Silby. *Physical Chemistry*, John Wiley, New York (1995).
- 3. I. N. Levine. *Physical Chemistry*, McGraw Hill, New York (2002).

CH-102 Chemistry-II Lab. (Cr. 1)

- 1. Determination of viscosity and parachor values of liquids.
- 2. Determination of percent composition of liquid solutions viscometrically.
- 3. Determination of refractive index and molar refractivity.
- 4. Determination of percent composition of liquid solutions by refractive index measurements.
- 5. Determination of molecular weight of a compound by elevation of boiling point (ebullioscopic method).
- 6. Determination of heat of solution by solubility method.

7. Determination of heat of neutralization of an acid with a base.

RecommendedBooks

- 1. Jaffar M., "Experimental Physical Chemistry", University Grants Commission, 1989.
- 2. Levitt B.P., "Findlay's Practical Physical Chemistry", 9th Ed., Longman Group Limited, 1978.
- 3. Shoemaker D., "*Experiments in Physical Chemistry*", 5th Ed., McGraw Hill Publishing Company Limited, 1989.

BS 2ndYear (Semester-III)

CH-201 Chemistry-III (Cr. 3)

Introduction to Organic Chemistry: Organic chemistry–the chemistry of carbon compounds; the nature of organic chemistry– a historical perspective.Localized and delocalized chemical bonding, concept of hybridization and shapes of organic molecules; resonance; aromaticity; tautomerism; hyperconjugation; hydrogen bonding.

Classes and Nomenclature of Organic Compounds: Classification of organic compounds; development of systematic nomenclature of organic compounds; IUPAC nomenclature of hydrocarbons and heteroatom functional groups including polycyclic system and compounds containing more than one functional groups.

Functional Group Chemistry: A brief introduction to the chemistry of hydrocarbons, alkyl halides, alcohols, phenols, ethers, aldehydes, ketones, amines, and carboxylic acids and their derivatives.

Applications of Chemistry: Use of organic compounds in industries, like medicinal, pharmaceutical, cosmetics, paints and pigments, polymers etc.

Pre-requisite: CH-101

RecommendedBooks

- 1. L.G. Wade, *Organic Chemistry*, 8thEd., Pearsons, 2012.
- 2. T.W. Graham Solomons and Graig B. Fryhle, *Organic Chemistry*, 10thEd., John Wiley & Sons, 2011.
- 3. J.G. Smith, *Organic Chemistry*, 3rdEd., McGraw-Hill Companies, 2012.
- 4. Brown and Foote, *Organic Chemistry*, 6thEd., Pearsons Publishers, 2011.
- 5. Stanley H. Pine, *Organic Chemistry*, 5thEd., McGraw-Hill, 2007.
- 6. D. Hellwinkel, Systematic Nomenclature of Organic Chemistry, Springer Verlag, 2001.

CH-201 Chemistry-III Lab. (Cr. 1)

- 1. Qualitative organic analysis: Systematic identification of organic compounds (monofunctional and simple bifunctional) and preparation of their derivatives.
- 2. Preparation of the following compounds: Suphanilic acid, dibenzyl acetone, methyl orange, dinitrobenzene from benzene, isolation of caffine.

- 3. Estimation of phenol (bromide-bromate method) and aniline (bromide-bromate and acetylation methods).
- 4. Equivalent weight of an acid (neutralization).
- 5. Identification of organic functional groups by I.R. spectroscopy.

Recommended Books

- 1. K.N. Williamson and K.M. Masters, *Macroscale and Microscale Organic Experiments*, published by Cengage learning, 2011.
- 2. J.J. Li, C. Limberakis and D.A. Pflum, *Modern Organic Synthesis in Laboratory*, OxfordUniversity Press, 2007.
- 3. J. Leonard, B. Lygo and G. Procter Nelson, *Advanced Practical Organic Chemistry*, Thomes Ltd. UK, 2001.

CH-202 Environmental Chemistry (Cr. 4)

Atmospheric Chemistry: The air around us, atmospheric temperature and pressure profile, Temperature inversion and photochemical smog, particulate matter in the atmosphere, Industrial pollutants, radioactivity, atmospheric aerosols, Acid rain –major sources, mechanism, control measures and effects on buildings and vegetation, Global warming – major green house gases, mechanism, control measures and global impact, The stratospheric ozone – the ozone hole, CFCs, ozone protection, biological consequences of ozone depletion.

Water Pollution and Water Treatment:Sources of water pollution-industrial sources and agricultural sources, heavy metals contamination of water, Eutrophification, detergents and phosphates in water, water quality criteria, Water purification – primary, secondary and advanced treatment, Removal of nitrogen and phosphorous compounds from polluted water, organic matter in water and its decomposition.

Soil Pollution: Soil and mineral resources, general principles of metal extraction, heavy metals contamination of soil, toxicity of heavy metals, bio-accumulation of heavy metals, organic matter in soil, macro- and micro-nutrients in soil, ion-exchange in soil, soil pH and nutrients availability.

Energy Production and Environment: Liquid and gaseous fuel, hydrogen economy.

Pre-requisite: CH-102

- 1. Collin Baird, *Environmental Chemistry*, W. H. Freeman and Company, New York, 1995.
- 2. John W. Moore and Elizabeth A. Moore, *Environmental Chemistry*, Academic Press Inc., New York, 1976.
- 3. Peter O. Neill, *Environmental Chemistry*, Chapman and Hall, London, 1993.
- 4. Derek M. Elsom, Atmospheric Pollution, Blackwell Publishers, Oxford, 1992.
- 5. Geoffrey Lean and Don Hinrichsen, *Atlas of the Environment*, Helicon Publishing Ltd., Oxford, 1992.
- 6. Anil Kumar De, *Environmental Chemistry*, Wiley Eastern Ltd. New Delhi, 1989.
- 7. Staneley E. Manahan, *Environmental Chemistry*, Brooks, California.

BS 2nd Year (Semester-IV)

CH-203 Chemistry-IV (Cr. 3)

Introduction to Analytical Chemistry:Chemical analysis, analytical processes, sampling and applications.

Measurements and Chemical Analysis: Concentration units, stoichiometric calculations.

Data Handling: Experimental errors, precision, accuracy and limits of detection, evaluation of data, quality of results, quality assurances and calibration methods.

Chemical Equilibria: Basic approach to chemical equilibria (acid-base, redox, complexation, precipitation), solubility and solubility product, ionic strength and activity coefficient, analysis by acid-based chemistry and titration curves.

Pre-requisite: CH-101

Recommended Books

- 1. Christian, G.D., "Analytical Chemistry", 6th Ed., John Wiley & Sons, New York, 2003.
- 1. Harris, D.C., "*Quantitative Chemical Analysis*", 8th Ed., Freeman, W.H. and Company, New York, 2011.
- 2. Skoog D.A., West D.M., and Holler F.J., "*Fundamentals of Analytical Chemistry*", 8th Ed., Thomson, 2004.

CH-203 Chemistry-IV Lab. (Cr. 1)

- 1. Lab safety and precautions
- 2. Introduction and calibration of glassware and instruments
- 3. Determination of Cations and anions (mass measurement)
- 4. Acid-base titrations
- 5. Redox titrations
- 6. Complexation titrations

Recommended Books

- 1. Vogel A.I., "A Textbook of Micro and Semi-micro Qualitative Inorganic Analysis", Longman Green & Co., 1995.
- 2. Jaffar M., "Experimental Physical Chemistry", University Grants Commission, 1989.

CH-204 Industrial Chemistry (Cr. 4)

Fundamentals of Chemical Industry: Basic principles and parameters for industrial plant location; Elementary treatment of general unit operations commonly used in industries such as size reduction; evaporation, filtration, distillation, crystallization and drying; Chemical unit processes like carbonation, sulfitation, defecation, nitration, etc. in chemical process industries.

Basic and Heavy Chemical Industries: Raw materials and chemicals; Flow sheet diagrams and commercial production of sulfuric acid, nitric acid, hydrochloric acid, caustic soda and washing soda; Applications of these chemicals in chemical industries. Industrial wastes and management.

Pre-requisite: CH-101 & CH-202

- 1. G.N. Pandey, A Text Book of Chemical Technology, 2nd Ed., Vikas Publishing house, 2000.
- 2. G.T. Auston, *Shreve's Chemical Process Industries*, 5th Ed., McGraw Hill Book Company Inc. New York, 1984.
- 1. E.R. Riegel, *Industrial Chemistry*, 5th Ed., Reinhold Publishing Corporation NewYork, 1997.
- 2. J.C. Kuriacase and J. Rajaran, *Chemistry in Engineering and Technology*, 2nd Ed., 1984.
- 3. Chuis A. Clauses III Guy Matison, *Principles of Industrial Chemistry*, 1978.
- 4. P.C. Jain, A Textbook of Applied Chemistry, 1993.
- 5. B.N. Chakrabarty, Industrial Chemistry, 1991.
- 6. H.L.White, Introduction to Industrial Chemistry, 1992.

BS 3rd Year (5th Semester)

CH-301 Analytical Chemistry-I (Cr. 3)

Electroanalytical methods: Classification, electrode processes, working principle, instrumentation and applications of potentiometry, coulometry, conductometry, amperometryand electrogravimetry. voltammetry: Basic principle, types, instrumentation and major applications; qualitative and quantitative aspects of voltammetry and polarography. Spectroscopy: Classification, basic principles, UV-visible spectroscopy, Lambert-Beer's lawand its deviations, major applications of UV-visible spectroscopy.

Recommended Books

- 1. G.D. Christian, *Analytical Chemistry*, 6thed., John Wiley & Sons Ltd.(2003).
- 2. D. Harvey, Modern Analytical Chemistry, McGraw-Hill Companies Inc.(2000).
- 3. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8thed., Thomson Books/Cole, Belmont, USA (2004).
- 4. D.A. Skoog, F.J. Holler and S.R. Crouch, *Principles of Instrumental Analysis*, 6thed., Thomson Brooks/Cole, USA (2007).
- 5. D.C. Harris, *Quantitative Chemical Analysis*, 5thed., W.H. Freeman Company, New York (1999).
- 6. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2nded., Wiley-VCH Verlag GmbH & Co. (2004).
- 7. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative chemical Analysis*, 6thed., Pearson Education Ltd. (2000).

CH-301 Analytical Chemistry Lab-I (Cr. 1)

- 1. Calibration of volumetric apparatus and analytical balance and to investigate errors in delivered quantity.
- 2. Determination of the concentration of strong acid solutions by conductometric titration.
- 3. Determination of the individual concentration of the acids in the given binary mixtures of strong/weak acidsby conductometric titration.
- 4. Evaluation of solubility product for lead iodate by conductance method.
- 5. Determination of solubility product of cadmium iodate titrimetrically.
- 6. Verification of the constancy of solubility product using solvent extraction.
- 7. Estimation of Ca^{2+} and Mg^{2+} concentration in drinking water by EDTA complexometric titration method.
- 8. Determination of the concentration of a strong/weak acid using potentiometric titration method.
- 9. Determination of Cl^{1-} and I^{1-} by the potentiometric titration method.
- 10. Establishment of the stoichiometric relation for the precipitation of silver chloride.
- 11. Preparation of buffer solutions and studying buffering capacity.

- 1. G.D. Christian, *Analytical Chemistry*, 6th ed., John Wiley & Sons Ltd. (2003).
- 2. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry, A Modern Approach to Analytical Science*, 2nd ed., Wiley-VCH Verlag GmbH & Co. (2004).

3. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, Vogel's Textbook of *Quantitative chemical Analysis*, 6thed., Pearson Education Ltd. (2000).

Inorganic Chemistry-I (Cr. 3) **CH-302**

Basic coordination chemistry: nomenclature, geometry of complexes, theories of Theory, V.B.T., C.F.T.), coordination compounds (Werner isomerism and stereochemistry, complex stability and factors affecting the stability, applications of coordination compounds. Classification of solvents: types of reactions in solvents, factors affecting physical and chemical properties of solvents, detailed study of liquid NH₃, liquid SO₂ and BF₃. Structure and energetics of inorganic molecules. Theory of metals and intermetallic compounds.

Recommended Books

- F.A. Cotton, et al., Advanced Inorganic Chemistry,6th ed., John Wiley, New York 1. (1999).
- G. Miessler and D.A. Torr. *Inorganic Chemistry*, 5th ed., Pearson-Printice Hall, 2. USA (2013).
- 3. J.E. Huheey, E.A. Keitlu and R.L. Keitlu, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Addison-Wesley, Reading (1997).
- A.J. Emeleus and A.G. Sharp, Modern Aspects of Inorganic Chemistry, Read K. 4. Paul,London, 3rd ed., Addison-Wessley Longmann, Inc., UK (1999).
- 5. T. Moeller, The Chemistry of the Lanthanides, Chapman and Hall Ltd. London (1965).
- J.D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall London, 5th ed., Wiley-6. Blackwell, UK (2008).

CH-302 Inorganic Chemistry Lab-I (Cr. 1)

- 1. Separation and estimation of pair of metal ions by paper chromatography, such as:
 - Cu^{2+}/Ni^{2+} i.
 - Al^{3+}/Fe^{3+} ii.
 - iii.
 - Ca^{2+}/Ba^{2+} Zn^{2+}/Pb^{2+} iv.
- Separation of halide ions by paper chromatography. 2.
- Estimation of Ag^{+1} and Cu^{2+} in given mixture using titration/precipitation method. 3.
- Estimation of Cu^{2+} and Ni^{2+} in given mixture using titration/precipitation method. 4.
- Estimation of Cu^{2+} and Pb^{2+} in given samplegravimetrically. 5.
- Estimation of Ba^{2+} and Ca^{2+} in given sample gravimetrically. 6.

- A.I. Vogel, A Textbook of Quantitative Inorganic Analysis: Theory and Practice, 1. Green and Co. Ltd., London (2000).
- 2. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, Vogel's Textbook of Quantitative chemical Analysis, 6thed., Pearson Education Ltd. (2000).

CH-303 Organic Chemistry-I (Cr. 3)

Structure-reactivity relationship: Changes in chemical reactivity with change in molecular structure in terms of acid base strength. Reactive intermediates: Types, structure, stability, methods of generation and reactivity. Introductory Stereochemistry: Historical background and significance; Chirality and stereoisomerism; Classification and nomenclature of stereoisomers; Drawing and interconversion of Fischer, Newman and Sawhorse projections. Chemistry of Hydrocarbons: General characteristics and common uses of aliphatic and aromatic hydrocarbons; Various strategies for the synthesis of hydrocarbons with emphasis on modern trends; Characteristic reactions of hydrocarbons and their importance in synthetic organic chemistry. Chemistry of Organohalides: General introduction; Methods of preparation and synthetic applications. Literature survey: Various sources of chemical literature and their scope.

Recommended Books

- 1. J.G. Smith, Organic Chemistry, McGraw-Hill, New York/Boston (2006).
- 2. L.G. Wade, Organic Chemistry, 5th ed., Pearson Education, Delhi(2003).
- 3. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, Boston (2007).
- 4. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, John Wiley & Sons (2007).
- 5. F.A. Carey, Organic Chemistry, McGraw-Hill, Higher Education, New York (2006).

CH-303 Organic Chemistry Lab-I (Cr. 1)

Experiments involving the synthesis of following classes of compounds and identification of the synthesized compounds by Physical (non-spectroscopic) and chemical methods:

- 1. Alkanes by coupling of alkyl halides.
- 2. Alkanes by decarboxylation of carboxylic acids.
- 3. Alkenes by dehydration of alcohols.
- 4. Alkenes by dehydrohalogenation.
- 5. Alkenes by pyrolysis of acetates.
- 6. Alkenes by Wittig reaction.
- 7. Alkynes by dehydrohalogenation of vicinal and geminal dihalides.
- 8. Alkynes by oxidation of dihydrazones of 1,2-diketones.
- 9. Aromatic Hydrocarbons by Friedel-Crafts alkylation.
- 10. Aromatic Hydrocarbons by Clemmenson and Wolff-Kishner reduction.
- 11. Grignard reagents (RMgX) from alkyl halides.
- 12. Reactions of RMgX.

- 1. A.M. Schoffstall and B.A. Gaddis, *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, (Druelinger, Melvin L.), McGraw-Hill, Boston (2004).
- 2. R. Adams, JR. Johnson and Wilcox Jr., *Laboratory Experiments in Organic Chemistry*, 6th ed., Collier-M, London (1970).
- 3. B.S. Furniss, *Vogel's Textbook of Practical Organic Chemistry Including Qualitative Organic Analysis*, Longman Group, London (1978).
- 4. H. Becker and I. Hazzard, *Organicum: Practical Handbook of Organic Chemistry*, Reading, Masachuse Addison-Wesley Publishing Co. (1973).
- 5. J.C. Gilbert, and S.F. Martin, *Experimental Organic Chemistry: A Miniscale and Microscale Approach*, SaundersCollege Publishing, Fort Worth (1998).

CH-304 Physical Chemistry-I (Cr.3)

Gases: Equation of stare for real gases, van der Waals equation, Virtual coefficients, Maxwell-Boltzmann law of molecular velocities (v_{rms} , v_{mp} , v_{av} , V_{rel}) and energies, transport properties. Thermodynamics: Applications of thermodynamic laws to chemical phenomena, spontaneity of chemical reactions, entropy, free energy (Gibbs and Helmholtz), free energy and concept of reversibility, heat capacity under different conditions, third law of thermodynamics. Chemical Kinetics: second- and third-order reactions rate equations for same and different initial concentrations, experimental determination of reaction's order, unimolecular and bimolecular reactions mechanisms, effects of catalysts on reaction rates, introduction to theories of reaction rates (collision theory and transition state theory (TST)). Electrochemistry and solutions: Ideal and nonideal solutions, ionic activity, ionic equilibria, redox reactions, developing electrochemical cells from redox reactions, Nernst equation, Phase diagram, Faradaic processes and nonfaradaic processes, electrochemical series.

Recommended Books

- 4. P. W. Atkins and J. de Paula, *Physical Chemistry*, 8th ed., Freeman & Co., New York (2006).
- 5. R. A. Alberty and R.J. Silby, *Physical Chemistry*, John Wiley, New York (1995).
- 6. I. N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).

CH-304 Physical Chemistry Lab-I (Cr.1)

- 1. Determination of equilibrium constant for the reaction $KI+I_2 \Longrightarrow KI_3$
- 2. Kinetic studies of the saponification of ethyl acetate.
- 3. Acid catalysed hydrolysis studies of sucrose.
- 4. Study of the adsorption isotherms of acetic acid-charcoal system.
- 5. Study of the charge transfer complex formation between iodine and benzene.
- 6. Determination of activation energy for acid catalysed hydrolysis of ethyl acetate.
- 7. Determination of partial molar volumes.
- 8. Characterization of the given compound by UV-Vis spectroscopy.

- 1. A.M. Halpern and G. C. Mcbane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd edition, W.H.Freeman (2006).
- 2. A.M. Helper, Experimental *Physical Chemistry: A Laboratory Textbook*. 2nd ed., Prentice Hall (1997).
- 3. J. Bassette, C. Denney, G.H. Jeffery and J. Mendham, *Vogel's Textbook of Quantitative Inorganic Analysis Including Elementary Instrumental Analysis*, English Language Book Society, 4th ed., (1978).
- 4. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative chemical Analysis*, 6thed., Pearson Education Ltd. (2000).
- 5. C. Garland, J. Nibler, D. Shoemaker, *Experiments in Physical Chemistry*, 8th Edition, McGraw Hill Higher Education (2008).

BS 3rd Year (6th Semester)

CH-311 Analytical Chemistry-II (Cr. 3)

Separation techniques: basic principle of solvent extraction, distribution coefficient, distribution ratio, counter current distribution, applications of solvent extraction. Theoretical aspects of chromatography: *Van Deemter* equation, column efficiency, band broadening and resolution, classification, various types of planar and column chromatography. Basic principles and applications of: adsorption, partition, ion exchange, size exclusion and affinity chromatography. Gas chromatography and high performance liquid chromatography: instrumentation, types of column, sample injection system, column loading and detectors, qualitative and quantitative aspects.

Recommended Books

- 1. D.A. Skoog,F.J. Holler and S.R. Crouch, *Principles of Instrumental Analysis*, 6thed., Thomson Brooks/Cole, USA (2007).
- 2. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 9thed., Thomson Books/Cole, Belmont, USA (2013).
- 3. D.C. Harris, *Quantitative Chemical Analysis*, 8thed., W.H. Freeman Company, New York (2010).
- 4. H.H. Willard, L.L. Merritt, J.A. Dean, F.A. Settle, *Instrumental Methods of Analysis*, Wiley, New York(2003).
- 5. G.D. Christian, Analytical Chemistry, 6thed., John Wiley & Sons Ltd. (2003).
- 6. D. Harvey, Modern Analytical Chemistry, McGraw-Hill Companies Inc.(2000).
- 7. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry, A Modern Approach to Analytical Science, 2nd ed., Wiley-VCH Verlag GmbH & Co. (2004).*
- 8. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, 6thed., Pearson Education Ltd.(2000).

CH-311 Analytical Chemistry Lab-II (Cr. 1)

- 1. Determination of Cu^{2+} in solution by electrogravimetric method.
- 2. Separation and quantification of copper in brass using constant-current electrolysis.
- 3. Verification of Beer's law and evaluation of molar extinction coefficient.
- 4. Estimation of Ni^{2+} in solution spectrophotometrically.
- 5. Spectrophotometric determination of ammonia.
- 6. Spectrophotometric determination of phosphate (PO_4^{3-}) in given sample.
- 7. Determination of Fe^{2+} by spectrophotometric method using 2,2'-bipyridine/ophenanthroline.
- 8. Spectrophotometric determination of Fe^{3+} with potassium thiocyanate.
- 9. Determination of distribution coefficient of a given solute between and aqueous/non-aqueous system.
- 10. Separation of $\dot{Fe^{3+}}$, Co^{2+} , Ni^{2+} and Cu^{2+} from mixture using paper and thin layer chromatography.
- 11. Determination of the percentage composition of Na₂CO₃ in commercial soda ash using pH titration method.
- 12. Estimation of Pb^{2+} ampereometrically through titration with potassium dichromate.
- 13. Determination of Ca^{2+} by the indirect titration with EDTA.
- 14. Determination of Zn^{2+} by direct titration with EDTA.

15. Analysis of commercial hypochlorite or peroxide by iodometric titration.

Recommended Books

- 1. G.D. Christian, Analytical Chemistry, 6thed., John Wiley & Sons Ltd.(2003).
- 2. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry: A Modern Approach to Analytical Science*,2nd ed., Wiley-VCH Verlag GmbH & Co.(2004).
- 3. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, 6thed., Pearson Education Ltd.(2000).

CH-312 Inorganic Chemistry-II (Cr. 3)

Chemistry of f-block elements (lanthanides, actinides): spectral and magnetic properties, oxidation states, electronic structure, lanthanide contraction, occurrence and extraction, major uses of lanthanides and actinides. Magnetochemistry: theory of magnetism, diamagnetism, paramagnetism, ferro-, ferri- and antiferromagnetism, magnetic susceptibility, measurement and instrumentation, magnetic moments. Spin cross over complexes: principle, types and applications. Effect of temperature on: magnetic properties of complexes, redox reactions, mechanisms of electron transfer reactions (outer sphere and inner sphere mechanisms). Balancing of chemical equations.

Recommended Books

- 1. F.A. Cotton, et al., *Advanced Inorganic Chemistry*,6th ed., John Wiley, New York (1999).
- 2. J.E. Huheey, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th ed., Addison-Wesley, Reading (1993).
- 3. M.C. Day Jr. and Jod Selbin, *Theoretical Inorganic Chemistry*, 2nded., Reinhold Publishing Corporation, New York (1969).
- 4. A.J. Emeleus and A.G. Sharp, *Modern Aspects of Inorganic Chemistry*, Read K. Paul, London (1983).
- 5. T. Moeller, *The Chemistry of the Lanthanides*, Chapman and Hall Ltd. London (1965).
- 6. T. Moeller, *The Chemistry of the Lanthanides:Pergamon Texts in Inorganic Chemistry*, Elsevier Science (2013).
- 7. J.D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall London (1996).

CH-312 Inorganic Chemistry Lab-II (Cr. 1)

- 1. Synthesis of selected coordination compounds such as:
 - i) $K_3[Cr(C_2O_4)_3]$
 - ii) $[Co(NH_3)_5Cl]Cl_2$
 - iii) $C_6H_4(OH)HgCl$
 - iv) $[Cu(NH_3)_4]SO_4$
 - v) $NH_4[Cr(SCN)_4(NH_3)_2].H_2O$
 - vi) Co(SCN)₂.3H₂O
- 2. Spectrophotometric determination of divalent metal ions in complexes using titration method.
- 3. Spectrophotometric determination of trivalent metal ions in complexes using titration method.
- 4. Separation of Fe^{2+}/Fe^{3+} and Zn^{2+} in a given sample by precipitation method.

- 5. Determination of Fe^{2+} by chloride extraction method.
- 6. Kinetic studies of inorganic chemical reactions such as iodine reaction with persulphate ion.

Recommended Books

- 1. A.I. Vogel, A Textbook of Quantitative Inorganic Analysis: Theory and Practice, Green and Co. Ltd., London (2000).
- 2. W.J. Jolly, *The Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, EnglewoodChiffes, New York (1970).
- 3. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, 6thed., Pearson Education Ltd.(2000).

CH-313 Organic Chemistry-II (Cr. 3)

General characteristics and common uses of: alcohols, phenols, ethers, aldehydes, and ketones and their thio-derivatives; Carboxylic acids and their derivatives; Amines; Nitriles; Cyanates; Nitro compounds. Methods of preparation: Reputed synthetic methods for the preparation of above functionalities including both classical and recent approaches. Chemical Reactivity: Characteristic chemical reactions of the above mentioned functionalities; Use of their chemical behavior to design multistep synthesis of some important products.

Recommended Books

- 1. T.W.G. Solomons and C.B. Fryhle, *Organic Chemistry*, John Wiley & Sons, New York (2014).
- 2. J. Clayden, N. Greeves, S.Warren and P. Wothers, *Organic Chemistry*, 2nd ed., Oxford University Press, New York (2012).
- 3. J.March, *Advanced Organic Chemistry*, 7th ed., John Wiley & Sons, New York (2013).
- 4. F.A.Carey, Organic Chemistry, 8th ed., McGraw-Hill, New York (2010).
- 5. G.M. Loudon, Organic Chemistry, OxfordUniversity Press, New York (2009).
- 6. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, Nelson Thornes, Cheltenham (2013).

CH-313 Organic Chemistry Lab-II (Cr. 1)

Organic preparations involving:

- 1. Dehydrohalogenation of alkyl halides.
- 2. Dehydration of alcohols.
- 3. Addition reactions of alkenes/alkynes.
- 4. Terminal alkynes as acids.
- 5. Diels-Alder reaction.
- 6. Aldehydes and ketones by oxidation of alcohols.
- 7. Reactions of stabilized carbanions from carbonyl compounds.
- 8. Conjugate addition to α , β -unsaturated ketones.
- 9. Reactions of Grignard reagents.
- 10. Preparation of carboxylic acids; esters and Fischer esterification.
- 11. Preparation of amides.
- 12. Preparation of amines.

Recommended books

- 1. D.L. Pavia, G.S. Kriz, G.M. Lampman and R.G. Engel, *A Microscale Approach to Organic Laboratory Techniques*, Brooks/Cole Laboratory Series for Organic Chemistry (2012).
- 2. A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry: A Text-book of Practical Organic Chemistry, 5th ed. (1996).
- 3. F.G. Mann and B.C. Saunders, *Practical Organic Chemistry*, Longman, London (1978).
- 4. J. Gilbert and S. Martin, *Experimental Organic Chemistry: A Miniscale and Microscale Approach*, Brooks Cole Laboratory Series for Organic Chemistry, 5th ed. (2010).
- 5. K. Williamson and K. Masters, *Macroscale and Microscale Organic Experiments*, Cengage Learning (2010).
- 6. D.W. Mayo, R.M. Pike, D.C. Forbes, *Microscale Organic Laboratory: with Multistep and Multiscale Syntheses*, John Wiley & Sons (2010).
- 7. S. Caron, *Practical Synthetic Organic Chemistry: Reactions, Principles and Techniques*, John Wiley & Sons, Inc., Hoboken, New Jersey (2011).
- 8. B.N. Campbell, Jr. and M.M. Ali, *Organic Chemistry Experiments: Microscale and Semi-Microscale*, Brooks/Cole (1994).
- 9. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, 3rd ed., CRC Press (2013).

CH-314 Physical Chemistry-II (Cr.3)

Quantum Chemistry: History and development of quantum mechanics, wave functions, Operators, eigen value equation, basics and postulates of quantum mechanics, Schrödinger's equation; quantitative mechanical model; particle in one-, two- and three-dimensional box, rigid rotator, simple harmonic oscillator, hydrogen and hydrogen like atoms. Chemical bonding: Molecular systems; H₂-molecule, molecular orbital and Valence bond theories, hybridization. Molecular Spectroscopy: Rotational and vibrational spectroscopy of di-atomic molecules, fundamentals of electronic spectroscopy.

Recommended Books

- 1. R.A. Albert, J.S. Robert and G.B. Moungi, *Physical Chemistry*, 4th ed., John Wiley and Sons (2004).
- 2. P.W. Atkins and J. de Paula, *Physical Chemistry*, 8th ed., Freeman & Co., New York (2006).
- 3. D.W. Ball, *Physical Chemistry*, 1st ed., Brooks/Cole Co. Inc. (2003).
- 4. B.R. Stephen, S.A. Rice and J. Roses, *Physical Chemistry*, 2nd ed., OxfordUniversity Press (2000).

CH-314 Physical Chemistry Lab-II (Cr.1)

- 1. Spectropotometric determination of Cu^{2+} in the given sample.
- 2. Conductometric determination of Cu^{2+} -EDTA mole ratio in the complex.
- 3. Separation of I_2 using solvent extraction method and to check the effectiveness of separation.
- 4. Determination of the molecular weight of a polymer by viscosity method.

- 5. Determination of the percentage composition of $KMnO_4/K_2Cr_2O_7$ in a given solution by spectrophotometry.
- 6. Evaluation of pK_a value of an indicator by spectrophotometric method.
- 7. Conductometric determination of hydrolysis constant (K_h) of conjugate base of a weak acid.
- 8. Determination of the rate of reaction of 2-chloro-2-methyl propaneby conductometric method.

Recommended Books

- 1. A.M. Halpern and G. C. Mcbane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd edition, W.H.Freeman (2006).
- 2. A.M. Helper, Experimental *Physical Chemistry: A Laboratory Textbook*. 2nd ed., Prentice Hall (1997).
- 3. J. Bassette, C. Denney, G.H. Jeffery and J. Mendham, *Vogel's Textbook of Quantitative Inorganic Analysis Including Elementary Instrumental Analysis*, English Language Book Society, 4th ed., (1978).
- 4. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative chemical Analysis*, 6thed., Pearson Education Ltd. (2000).
- 5. C. Garland, J. Nibler, D. Shoemaker, *Experiments in Physical Chemistry*, 8th Edition, McGraw Hill Higher Education (2008).

Specialization (Inorganic-Analytical/Organic/Physical Chemistry) BS 4th Year (7th& 8th Semester)

Inorganic/Analytical Chemistry

CH-401 Molecular Spectroscopy (Cr. 3)

Molecular structure and spectral transitions: Measurement of spectra, light scatteringelastic and inelastic, absorption and emission spectroscopy. Absorption spectroscopy in UV-Visible region: Absorbance and transmittance, spectral resolution and errors in concentration measurements, applications and comparison of fluorescence and phosphorescence spectroscopy, spectral interferences and spectra of mixtures, chemical interferences, instrumental interferences. Instrumentation: Wavelength separations, sources and detectors for electromagnetic radiations. Derivative spectroscopy: Theory and applications. IR and Raman spectroscopy: Vibrational frequencies, qualitative analysis, IR spectra and Raman spectra, band intensities, quantitation, IR and Raman spectrophotometers, correlation charts and tables. NMR Spectroscopy: Introduction, principles and applications of NMR.

- 1. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc.(2000).
- 2. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2nded., Wiley-VCH, Verlag GmbH & Co. KGaA, Weinheim (2004).
- 3. D.L. Pavia, G.M. Lampman, and G.S. Kriz, *Introduction to Spectroscopy*, 3rded., Thomson Learning Inc.(2001).
- 4. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA(2000).

- 5. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6thed., Pearson Education Ltd.(2000).
- 6. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8thed., Thomson Books/Cole, Belmont, USA (2004).
- 7. F. Rouessac and A. Rouessac, *Chemical Analysis Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).
- 8. G.D. Christian, *Analytical Chemistry*, 6thed., John Wiley & Sons Ltd., Singapore(2003).
- 9. D.C. Harris, *Quantitative Chemical Analysis*, 5thed., W.H. Freeman Company, New York (1999).

CH-402 Atomic Spectroscopy (Cr. 3)

Origin of spectral transitions in atoms: Atomic spectra and spectral notations, intensities and line widths of gas-phase atomic spectra and its variations with temperature and pressure. Absorption & emission spectra: Boltzman distribution, spectral line broadening, background correction, factors affecting atomization. Atomic absorption and emission methodologies: Optimization of analytical conditions, concentration ranges in atomic spectroscopy. Spectral, physical, chemical and instrumental interferences and their elimination. Optical components of atomic absorption/emission spectrophotometers: Radiation sources, atomizers, monochromators and detectors, modulation in atomic spectroscopy. Flame Vs. Electrothermal atomic absorption spectroscopy: Qualitative and quantitative applications of absorption and emission measurements. Flame photometry: Flame characteristics and spectral interferences, components of flame photometer, nonmetals and flame photometry. Sample and standard preparation methods for atomic spectroscopy.

Recommended Books

- 1. F. Rouessac and A. Rouessac, *Chemical Analysis Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).
- 2. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA (2000).
- 3. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2nded., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).
- 4. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, Fundamentals of Analytical Chemistry, 8thed., Thomson Books/Cole, Belmont, USA (2004).
- 5. R.D. Braun, *Introduction to Instrumental Analysis*, McGraw-Hill Book Company (1987).
- 6. E.H. Evans, *An Introduction to Analytical Atomic Spectrometry*, John Wiley & Sons Ltd., New York (1998).
- 7. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4thed., SaundersCollegePublishing, USA (1992).
- 8. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6thed., Pearson Education Ltd.(2000).

CH-403 Organometallic Chemistry (Cr. 3)

Introduction: historical background and current trends. 18-Electron rule: rationalization, limitations. Types of ligands. Chemistry and bonding of metal-sigma and pi-complexes: metal carbonyls and related compounds, metal alkyls, metal hydrides, complexes of

molecular nitrogen, oxygen and hydrogen, metal phosphines and complexes of pi-bond ligands. Applications of organometallic chemistry. Metal cluster and rationalization of their structures: electron counting schemes in clusters.

Recommended Books

- 1. R.H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, John Wiley & Sons (2014).
- 2. M. Bockmann, Organometallic Chemistry 1 & 2, Oxford Chemistry Primers (1994).
- 3. A. Yamamoto, Organotransition Metal Chemistry: Fundamental Concepts and Applications, John Wiley & Sons (1986).

CH-404 Crystallography (Cr. 3)

Introduction: Techniques involving X-rays, historical background, the eye and microscope analogy, interatomic on intermolecular forces, solid-crystalline, amorphous. X-rays: Production, X-ray tubes, absorption and filtering, selection of radiation, detection of X-rays. Geometry of the crystal: Introduction, unit cells, lattices, crystal systems, crystal classes, space groups. Symmetry: Macroscopic and microscopic symmetry elements, crystal symmetry and properties. Diffraction of X-rays: Bragg's equation and Bragg's law, reciprocal lattice, Bragg's law in reciprocal lattice. Diffractional methods: Powder methods – camera and diffractometer, single crystal methods – camera (Rotation, Oscillation, Weissenberg and Precession) and diffractometer. Intensities of the diffracted beam; measurement, data reduction. Solution of the structure, refinement and interpretation of the result.

Recommended Books

- 1. B.D. Culity and S.R. Stock, *Elements of X-ray Diffraction*, 3rd ed., Prentice Hall (2003).
- 2. L. Smart and M. Gagan, *The Molecular World: The Third Dimensions*, RSC, UK (2002).
- 3. J.P. Glusker, *Crystal Structure Analysis for Chemists and Biologists*, Wiley-VCH (1994).

CH-405 Inorganic Polymers (Cr. 3)

Introduction: Classification, polymerization processes. Preparation and properties of: polysiloxanes, polyphosphazenes, polythiazyl and transition-metal polymers. Characterization of polymeric materials: molecular weight determination, IR and NMR spectroscopy, thermogravimetry, dynamic mechanical analysis, microscopy, differential scanning calorimetry. Applications of polymers.

- 1. J.E. Mark, H. R. Allcock and R. West, *Inorganic Polymers*, Oxford University Press, (2005).
- 2. F.G.A. Stone and W.A.G. Graham, *Inorganic Polymers*, Academic Press, Inc., London (1962).
- 3. F.G.R. Gimblett, *Inorganic Polymer Chemistry*, Butterworths, London (1963).
- 4. C.E. Carraher, Jr., J.E. Sheads and C.U. Pittman, Jr., *Advances in Organometallic and Inorganic Polymer Science*, Marcel Dekker, Inc., New York (1982).

5. C.E. Carraher, Jr., *Polymer Chemistry*, 5th ed., Marcel Dekker, Inc., New York (2000).

CH-406 Group Theory in Chemistry (Cr. 3)

Introduction: symmetry; operations & elements, point groups, crystallographic and noncrystallographic point groups, assigning point groups, definition and properties of a group, subgroups, group multiplication table, matrix representation of a group, character tables. The great orthogonality theorem, rules derived from the theorem, developing of character tables for various point groups, matrices, matrix multiplication, character of a matrix, reducible representations and their reduction, symmetry and physical properties of molecules. Application of group theory: to valence bond theory and hybrid orbitals, crystal field theory and John-Teller distortion, MXn molecules with pi-bonding, pi-bonding in aromatic ring systems, vibrational spectroscopy, molecular vibrations using internal coordinates, bonding modes, geometric isomers, infrared and Raman active vibrations, exclusion rule, molecular orbital diagrams, metal sandwich compounds and AB_n molecules.

Recommended Books

- 1. K.C.Molloy, *Theory for Chemists: Fundamental Theory and Applications*, 2nd Ed., Woodhead Publishing in Materials (2011).
- 2. L.R. Carter, *Molecular Spectrometry and Group Theory*, John Wiley and Sons (2004).
- 3. A. Vincent, *Molecular Symmetry and Group Theory*, 2nd Ed., Wiley (2000).
- 4. F.A. Cotton, *Chemical Applications of Group Theory*, 3rd Ed., Wiley India (2008).
- 5. A.B.P. Lever, *Introduction to Electronic Spectroscopy*, 2nd Ed., Elsevier, Amsterdam (1984).

CH-407 Chemical Process Industries (Cr. 3)

Basic data for the development of the industrial unit. Chemistry and technology of various industries: Water conditioning, cement, glass, ceramics, leather, fertilizers, sugar and starch, glue and gelation, pulp and paper, soap and detergent, oils, fats and waxes, rubber and plastics.

Recommended Books

- 1. G.T. Austin, *Shreeve's Chemical Process Industries*, 5th ed., McGraw-Hill Book Company, New York (1995).
- 2. K.H. Davis, F.S. Berner and S.C. Bhatia, *Handbook of Industrial Chemistry*, Vol. I & II, C.B.S. Publisher & Distributor, New Delhi (2004).
- 3. C.C. Furnas, *Roger's Industrial Chemistry*, Vol. I & II, D. Van Nostrand Company, New York (1950).

CH-408 Nuclear Methods of Analysis (Cr. 3)

Radioactivity and nuclear reactions: sources of nuclear bombarding particles, detection and measurement of nuclear radiation, effects of radiation on biological systems. Nuclear techniques and applications of: Neutron activation analysis, isotope dilution method, radio-immuno assays, carbon-14 dating. Mössbauer spectroscopy: basic principles, instrumentation and application in various fields.

Recommended Books

- 1. D.A. Shoog, F.J. Holler and S.R. Crouch, *Principles of Instrumental Analysis*, 6th Ed., Thomson Brooks/Cole (2007), USA (Indian Ed.).
- 2. G. Ghoppin, J.O. Liljenzin and J. Rydberg, *Radiochemistry and Radiochemistry*, 3rd Ed., Butterworth Heinemann (2002).
- 3. K.H. Lieser, Nuclear and Radiochemistry: Fundamentals and Applications, 2nd Ed. (Revised), Wiley-VCH, Berlin (2001).
- 4. G. Choppin, J.O. Liljenzin and J. Rydberg, *Radiochmistry and Nuclear Chemistry*, 3rd ed., Butterworth-Heinemann (2002).
- 5. Y. Hido and M. Satake, *An Introduction to Nuclear Chemistry*, Discovery Publishing House, New Delhi (2003).
- 6. G. Friedlander and J.W. Kennedy, *Nuclear Radiochemistry*, 3rd ed., John Wiley and Sons, New York (1981).

CH-409 Coordination Chemistry (Cr. 3)

Overview: Historical developments, preparation and reactions of coordination compounds in aqueous and non-aqueous solvents, thermal dissociation of solid complexes. Complex stability: factors, thermodynamics and stability constant. Kinetics and mechanisms: basic kinetic parameters, inert and labile complexes of coordination compounds. Mechanisms of substitution reactions: Dissociation, association and interchange reaction pathways. Octahedral substitution reactions: Dissociation, associative, the conjugate base mechanisms. chelating effect. Square planar substitution reaction: Kinetic Stereochemistry, trans effect. Oxidation-reduction reactions: Inner and outer sphere reaction mechanisms. Organometallics and their role in catalysis, comparative studies of coordination compounds belonging to main group and transition elements with reference to synthesis and stability. Intermetallic compounds.

Recommended Books

- 1. G.L. Miessler and D.A. Tarr, *Inorganic Chemistry*, 5th ed., Pearson Education International (2013).
- 2. F. Basolo and R.C. Johnson, *Coordination Chemistry*, NBF Pakistan (1988).
- 3. J.E. Huheey, *Inorganic Chemistry, Principles of Structure and Reactivity*, 4th ed., Addison-Wesley, Reading/Singapore (1993).
- 4. F.A. Cotton, et al., *Advanced Inorganic Chemistry*, 6th ed., John Wiley, New York (1999).
- 5. P.L. Soni and V. Soni, *Coordination Chemistry: Metal Complexes*, CRC Press, Taylor& Francis (2013).

CH-410 Nano Materials in Chemistry

Nanoscale materials: Introduction, size comparison of nanoparticles with condensed matter, classification, metal oxides, sulfides, nitrides, fullerenes, graphenes, graphite, diamond, activated carbon, pyrolytic carbon, structure and bonding in nanomaterials. Nanostructure-dependent properties: electrical, magnetic, optical and catalytic. Synthesis, characterization and functionalization of nanomaterials for advanced applications.

Recommended Books

1. K.J. Klabundle,R.M. Richards, *Nanoscale Materials in Chemistry*, John Wiley & Sons, Inc., New York, 2nd edition, (2009).

- 2. A.A. Moosa, *Carbon Nanotubes: Synthesis and Applications*, Dar Djlah Publishing, Amman, Jordan (2012).
- 3. G. A. Ozin, A. C. Arsenault, L. Cademartiri, *Nanochemistry: A Chemical Approach to Nanomaterials*, Royal Society of Chemistry (2009).

Note: In the VII semester the student shall have to take either CH-491 Or CH-497 course, whichever is offered by the department.

CH-491 Inorganic/Analytical Chemistry Laboratory-III (Cr. 3)

Note: Any eight practical will be performed subject to availability of chemicals and instruments.

- 1. Preparation and characterization of di- and tribenzyltin chloride.
- 2. Preparation and analysis of clathrate compound (benzene ammine nickel cyanide), Ni(CN)₂.NH₃.C₆H₆.
- 3. Synthesis and characterization of inorganic compounds [Co(NH₃)₅Cl], [Co(NH₃)₅NO₂].
- 4. Preparation and estimation of Grignard's reagent, C₂H₅MgBr.
- 5. Synthesis and characterization of acetylacetonato metal complexes.
- 6. Synthesis and characterization of triphenyltin and tetraphenyltin chloride.
- 7. Preparation of inorganic compounds and study of their optical activity, $d_1[$ trisethylenediamine Co(III) $]I_3$.
- 8. Water quality evaluation by measurement of the physicochemical parameters in drinking water.
- 9. Chemical analysis of Portland cement.
- 10. Determination of percentage composition of copper and zinc in Brass.
- 11. Spectrophotometric determination of Pb^{2+} using solvent extraction.
- 12. Spectrophotometric determination of NO_3^{1-} nitrogen in water.
- 13. Spectrophotometric determination of aspirin, phenacetin and caeffiene (APC) tablets using solvent extraction.
- 14. Qualitative and quantitative analysis of fruit juices for vitamin C using HPLC.

Recommended Books

- 1. W.J. Jolly, *The Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, EnglewoodChiffes, New York (1970).
- 2. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative chemical Analysis*, 6th ed., Pearson Education Ltd. (2000).
- 3. G.D. Christian, Analytical Chemistry, 6th ed., John Wiley (2003).

Or

CH-497 Thesis/Research Project in Inorganic/Analytical Chemistry (Cr. 3)

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

Note: In the VIII semester the student shall have to take either CH-494 Or CH-500 course, whichever is offered by the department.

CH-494 Advanced Inorganic/Analytical Chemistry Laboratory (Cr. 3)

The course teacher(s) shall offer advanced level practical's involving different experimental facilities available in the section/department. The details of the laboratory work and the equipment involved shall be decided by the teacher concerned on the basis of the courses taught.

Or

CH-500 Thesis/Research Project in Inorganic/Analytical Chemistry (Cr. 3)

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

Organic Chemistry

CH-421 Chemistry of Heterocycles (Cr. 3)

Heterocycles: Introduction, significance and uses. Nomenclature: IUPAC nomenclature of monocyclic, bicyclic and bridged heterocyclic systems containing one, two and three heteroatoms. Synthesis and reactions: Three-seven membered nitrogen, oxygen and sulfur containing heterocycles with one, two and three heteroatom; Fused ring heterocycles: quinoline, isoquinoline, coumarin, chromone, indole, benzo[b]thiophene, benzo[b]furan, isoindole, benzo[c]thiophene, isobenzofuran, benzimidazole, benzothiazole, benzoxazole, indazole, 1,2-benzisothiazole and 1,2-benzisoxazole.

Recommended Books

- 1. L.D. Quin and J.A. Tyrell, *Fundamentals of Heterocyclic Chemistry*, Wiley & Sons (2010).
- 2. R.K. Bansel, *Heterocyclic Chemistry*, 4th ed., New Age International Pvt. Ltd., India (2005).
- 3. T. Eicher and S. Hauptmann, *The Chemistry of Heterocycles*, 2nd ed., George Thieme Verlag, New York (2003).
- 4. J.A. Joule, K. Mills and G.F. Smith, *Heterocyclic Chemistry*, Stanley Thomes Publications. Ltd. (1998).
- 5. R.H. Acheson, *An Introduction to Chemistry of Heterocycles*, John Wiley, New York (1987).
- 6. G.M. Loudon, *Organic Chemistry*, 4th ed.,OxfordUniversity Press, New York (2002).
- 7. M.A. Fox and J.K. Whitesell, *Organic Chemistry*, 3rd ed., Jones and Bartlett, Boston (2003).
- 8. M. Samisburg, *Heterocyclic Chemistry*, Royal Society of Chemistry (2001).

CH-422 Reaction Mechanism-I (Cr. 3)

Introduction to reaction mechanism: Basic concepts; Energy profile diagrams; Intermediate *vs* transition state; The Hammond postulate; Microscopic reversibility; Kinetic and thermodynamic requirement; Kinetic and thermodynamic control; Significance of reaction mechanism. Determination of reaction mechanism: Identification of products: testing possible intermediates and trapping of intermediates; Isotopic labeling and isotope effects; Catalysis; Stereochemical and kinetic studies. Mechanisms of different types of reactions: Aliphatic nucleophilic substitution reactions: S_N1 , S_N2 , S_Ni S_N1' , S_N2' , S_Ni' and neighboring group mechanisms; Aliphatic electrophilic substitution reactions: S_E1 and SET mechanisms; Aromatic electrophilic substitution reactions: the arenium ion mechanism; Aromatic nucleophilic substitution reactions: S_NAr , S_N1 , benzyne and $S_{RN}1$ mechanisms; Addition reactions across C-C and C-X heteroatom multiple bonds; Elimination reactions: E1, E2, E1cB mechanisms; Saytzeff and Hoffman rules; Structure and reactivity effects.

- 1. R. Bruckner and M. Harmata, *Reaction Mechanisms, Reactions, Stereochemistry and Synthesis*, Springer Verlag (2010).
- 2. R.P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th ed., Longman Scientific & Technical, London (1986).

- 3. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, John Wiley&Sons, New York (2007).
- 4. B.K. Carpenter, *Determination of Organic Reaction Mechanisms*, John Wiley & Sons, New York (1984).
- 5. T.H. Lowry and K.W. Richardson, *Mechanism and Theory in Organic Chemistry*, Harper & Row Publishers, New York (1987).
- 6. Jacobs, *Understanding Organic Reaction Mechanisms*, The University Press, Cambridge (1997).
- 7. J.Clayden, N.Greeves, S. Warren and P.Wothers, *Organic Chemistry*, OxfordUniversity press 2001.
- 8. M.G. Moloney, *Reaction Mechanisms at a Glance: a Stepwise Approach to Problem-Solving in Organic Chemistry*, Blackwell Science, Oxford (2000).
- 9. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanisms*, Harcourt Science, San Diego (2002).

CH-423 Spectroscopic Methods in Organic Chemistry-I (Cr. 3)

Introduction: The electromagnetic spectrum; Units and their interconversion; The absorption of electromagnetic radiation by organic molecules. Molecular formula and its determination: Molecular mass determination; Rule of thirteen and molecular formula; Index of hydrogen deficiency. UV-Visible spectroscopy: Introduction; Theory; Sample handling and instrumentation; Chromophores: Conjugated dienes, trienes, polyenes, unsaturated carbonyl compounds, benzene and its derivatives, polynuclear aromatic hydrocarbons and diketones; Factors affecting absorption maxima; Empirical rules for calculation of lambda-max; Applications of UV-visible spectroscopy. Infra Red spectroscopy: Introduction; Theory; Sampling techniques; Instrumentation; Characteristics of vibrational frequencies of functional groups; Interpretation of IR spectra. Mass spectrometry: Introduction; Theory; Types of fragments: odd electron and even electron containing neutral and charged species; Nitrogen rule; Isotopic peaks; Meta-stable ion peaks; Sample handling; Instrumentation; Fragmentation patterns in different classes of organic compounds; Interpretation of mass spectra. Applications of organic molecules based on UV-visible, IR and MS data.

- 1. R.M. Silverstein, F.X. Webster and D.J. Kiemle, *Spectrometric Identification of Organic Compounds*, John Wiley & Sons Inc., USA (2005).
- 2. D.L. Pavia, G.M. Lampman and G.S. Kriz, *Introduction to Spectroscopy: a Guide for Students of Organic Chemistry*, Thomson Learning, Australia (2001).
- 3. D.W. Brown, A.J. Floyed and M. Sainsbury, *Organic Spectroscopy*, I. Wiley and Sons, Chichester (1998).
- 4. D.H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4th ed., McGraw-Hill Book Co., London (1987).
- 5. M. Hesse, H. Nleir and U. Zech, *Spectroscopic Methods in Organic Chemistry*, Georg Thiemc, Stuttgart, New York (1997).
- 6. Y.C. Ning, Spectral Identification of Organic Compounds with Spectroscopic Techniques, Wiley-VCH, Weinheim (2005).
- 7. M. Younas, Organic Spectroscopy, Ilmi Kitab Khana, Lahore (2004).

CH-424 Chemistry of Natural Products (Cr. 3)

Introduction: Primary and secondary metabolites; Importance of natural products; Classification and biosynthesis of natural products including fatty acids, flavonoids, terpenoids, steroids and alkaloids. Isolation: General isolation scheme of natural products; Specific isolation strategies for fatty acids, flavonoids, terpenoids, steroids and alkaloids. Structure elucidation: Classical and modern techniques for structure elucidation of natural products: Examples of classical and modern syntheses of natural products for fatty acids, flavonoids, terpenoids, steroids and alkaloids.

Recommended Books

- 1. J. Clayden, N. Greeves, S. Warren and P. Worthers, *Organic Chemistry*, OxfordUniversity (2001).
- 2. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, *Natural Products*, Longman Group Ltd., U.K. (1994).
- 3. K.C.Nicolau, J. S. Chen, *Classics in Total Synthesis III*, VCH, Weinheim (2011).
- 4. I.L. Finar, Organic Chemistry: Stereochemistry and the Chemistry of Natural *Products*, Vol. 2, Pearson Education, Delhi (1975).
- 5. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd ed., Chapman Hall, London (1993).
- 6. K. Nakanishi, T. Goto, S. Ioto, S. Natori, S. Nozone, et al., *Natural Products Chemistry*, Vol. 1, Academic Press Inc, New York (1974).

CH-425 Biochemistry (Cr. 3)

Introduction: Significance of biochemical reactions. Carbohydrates: Classification; The structure and configuration of glucose and fructose; Anomeric forms; Structure, function and metabolism of monosaccharides, glycosides, disaccharides, trisaccharides and polysaccharides. Proteins and Amino acids: Proteins; Amino acid structure and chemistry; α-Amino acids; Synthesis and reactions of amino acids; Peptide synthesis; Protein structural levels (primary, secondary, tertiary, super-tertiary and quaternary); Composition and features; Protein denaturation; Solid-phase chemical synthesis; Metabolism of proteins. Enzymes: Classification; Nomenclature and types; Functions of cyclooxygenase (COX), lipoxygenase (LOX), carbonic anhydrases (CAs), acetylcholinesterase (AChE) and reverse transcriptase (RT); Isozymes: kinetics, mechanism of action and enzyme inhibition. Nucleic acids: Polynucleotides; Nucleosides; Nucleotides; Deoxynucleotides; Pentose sugar (ribose and deoxyribose); Nucleobases; Deoxyribonucleic acid (DNA): structure and types; Ribonucleic acid (RNA): types and functions. Primary, secondary and tertiary structures; Drug-DNA interaction; Binding modes: covalent bonding, intercalation mode, groove binding mode and electrostatic binding mode; Metabolism of nucleic acids. Lipids: Fatty acids; Fats and oils (triglycerols); Icosanoids (prostaglandin, prostacyclins, thromboxanes, lipoxins and leukotrienes); Glycerophospholipids; Sphingolipids; Glycolipids; Steroids; Waxes, soaps and detergents; Lipid soluble vitamins; Metabolism of lipids.

- 1. D. Voet and J. Voet, *Biochemistry*, 2nd ed., John Wiley, New York (1995).
- 2. I.L. Finar, Organic Chemistry, (Stereochemistry and the Chemistry of Natural Products), Vol. II, Pearson Education, New Delhi (1975).

- 3. C.K. Mathews, K.E. van Holde, K.G. Ahern, *Biochemistry* 3rd ed. (International Ed.) San Francisco, Calif. : Addison-Wesley (2000).
- 4. T. Delvin, *Textbook of Biochemistry*, 4th ed., John Wiley, New York (1997).
- 5. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, *Natural Products*, Longman Group Ltd., U.K. (1994).
- 6. M. Hem, L.R. Best and S. Pattison, *Introduction to General, Organic, and Biochemistry*, Susan Arena, Wiley (2004).
- 7. D. Voet and J.G. Voet, *Fundamentals of Biochemistry: Life at the Molecular Level*, Charlotte W. Pratt, Wiley (2005).
- 8. F.A. Bettelheim, W.H. Brown and M.K. Campbell, *Introduction to General, Organic and Biochemistry*, Shawn O. Farrell, Brooks Cole (2006).
- 9. R. Garrett and C.M. Grisham, *Biochemistry*, Belmont, CA : Brooks/Cole, Cengage Learning (2013).

CH-426 Name Reactions (Cr. 3)

History of named reactions, description of the primary contributor associated with discovery and development of the reaction with seminal references, currently accepted mechanism and applications in organic synthesis for the following organic named reactions: Acyloin condensation, alkene metathesis, Arbuzov reaction, Bamford-Stevens-Shapiro olefination, Baylis-Hillman reaction, Corey-Bakshi-Shibata reduction, Corey-Fuchs alkyne synthesis, Doering-Laflammeallene synthesis, Finkelstein reaction, Glaser coupling, Henry reaction, Krapcho reaction, Ley oxidation, Mitsunobu reaction, Mukaiyamaaldol reaction, Pausin-Khand reaction, Peterson olefination, Prins reaction, Robinson annulations, Seyferth-Gilbert homologation, Simmons-Smith cyclopropanation, Vilsmeier-Haackformylation and Yamaguchi lactonization.

Recommended Books

- 1. L. Kurti and B. Czako, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Academic Press (2005).
- 2. B. P. Mundy, M. G. Ellerd and F. G. Favaloro Jr., *Named Reactions and Reagent in Organic Synthesis*, 2nd Ed. Wiley Interscience, New Jersy (2005).
- 3. T. Laue and A. Plagens, (translated by C. Vogel), *Named Organic Reactions*, 2nded., John Wiley and Sons, Ltd. West Sussex (2005).
- 4. E. J. Corey and J. J. Li, *Named Reactions for Functional Group Transformations*, Wiley New York(2007).
- 5. A.Hassner and C. Stumer, *Organic Syntheses Based on Name Reactions and Unnamed Reactions*, Pergamon Press (1994).

CH-427 Organic Polymer Chemistry (Cr. 3)

Basic concepts, Nomenclature, classification of polymers. Polymer synthesis: Step growth, chain growth, free radical and ionic polymerizations; Ziegler-Natta polymerization; Co-polymerization. Characterization of polymers: Molecular weight determination using chemical and physical methods such as end group analysis, gel permeation chromatography, viscosity and osmometry; Thermal methods such as differential scanning calorimetry and thermal gravimetric analysis; Spectroscopic methods such as infra red and nuclear magnetic resonance; Thermo-mechanical methods.Uses and applications: Examples of uses of polymers in various fields such as electrical, electronic, biomedical and engineering.

Recommended Books

- 1. F.W. Billmeyer, *Textbook of Polymer Science*, Interscience (1994).
- 2. G. Odian, *Principles of Polymerization*, 3rd ed., John Wiley & Sons (2004).
- 3. C.E. Carrahers, *Carraher's Polymer Chemistry*, 9th ed., CRC Press (2013).
- 4. H.R. Allcock and F.W. Lampe, *Contemporary Polymer Chemistry*, 4th ed., Prentice Hall (2003).
- 5. M.S. Bhatnagar, A Textbook of Polymers, Vol. I, II, III, S. Chand & Co. Ltd. (2004).
- 6. J.R. Fried, *Polymer Science & Technology*, Prentice Hall, Inc. (1995).
- 7. M.P. Stevens, *Polymer chemistry: An Introduction*, Oxford University Press (1999).
- 8. P.S.Malcolm, *Polymer Chemistry*, OxfordUniversity Press (2005).

CH-428 Reaction Mechanism-II (Cr. 3)

Rearrangements: Reactions involving 1,2 and non-1,2 rearrangements and their mechanisms; Classification: nucleophilic, electrophilic and radical rearrangements; Mechanism: general mechanism and migratory aptitude with examples; Stereochemistry: stereochemical considerations in rearrangement reactions with respect to migrating group, migratory origin and migratory terminus; Examples: pinacol, benzyl-bezilic acid, Baeyer-Villiger, Hoffmann, Curtius, Schmidt, Lossen, Bekmann, Arndt Eistert, Favorskii, Quasi-Favorskii, Stevens, Hydride shifts and Diene-Phenol rearrangements. Oxidations: Reactions involving removal of hydrogen, cleavage of C-C bond, replacement of hydrogen by oxygen, addition of oxygen and oxidative coupling along with their mechanisms; Selectivity: chemo- and stereoselectivity; Oxidizing agents: Cr based reagents, e.g., chromic acid, Jones, Collins, PCC and PDC; Mn based oxidation; activated sulfoxide based oxidation including Moffat, Goldman, Doering and Swern oxidation; Hypervalent iodine based oxidation including IBX and Dess-Martin periodinane; Radical based oxidation, e.g., TEMPO oxidation; Mn and Os based dihydroxylation; Sharpless dihydroxylation; V, Ti, Mn, dioxirane and peracid based epoxidation; Periodate and ozone based alkene oxidative cleavage. Reductions: Reactions involving replacement of oxygen by hydrogen, removal of oxygen, reductive cleavage and reductive coupling and their mechanism; Selectivity: chemo- and stereoselectivity; Reduction reactions: hydrogenation reaction, metal hydride as reducing agents and their variations, dissolving metal reduction, Wolf-Kishner and Clemmenson reduction. Pericyclic Reactions: Introduction and significance; Classification: signatropic rearrangement, electrophilic and cycloaddition reactions; Mechanistic aspects: Woodward-Hoffmann rule and frontier orbitals method; Primary and secondary orbital interactions and the Alder rule; Photochemical and thermal pericyclic reactions; Conrotatory and disrotatory processes; Ene reaction; Selectivity: region- and stereoselectivity.

- 1. F.A. Carey and R.J. Sundberg, *Advance Organic Chemistry, Part B. Reaction and Synthesis*, 4th Ed. Kluwer Academic/Plenum Publishers, New York (2000).
- 2. J. March, Advanced Organic Chemistry: Reaction, Mechanism and Structure, 5th ed., John Wiley, New York (2007).
- **3.** F. L. Ansari, R. Quershi and M.L. Quershi, *Electrocyclic Reactions*, John Wiley & Sons (1999).
- 4. R.O.C. Norman, *Principles of Organic Synthesis*, 3rd ed., Chapman and Hall, London (1993).

- 5. R.T. Morrison and R.N. Boyd, *Organic* Chemistry, 6th ed., Prentice Hall, New Jersey (1992).
- 6. P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th ed., Longman Scientific and Technical, London (1986).

CH-429 Stereochemistry (Cr. 3)

Types of Chirality: Central, axial and planar chiral compounds; Atropisomers; Molecular overcrowding and cyclostereoiosomerism. Static stereochemistry: Symmetry elements and symmetry operations; Point group classification; Methods for determination of relative and absolute configuration. Dynamic stereochemistry: Prostereoisomerism and prochirality; Conformations and energy diagrams; Stereochemistry in addition, elimination and nucleophilic substitution reactions. Analytical methods for determination of stereoisomeric composition: chromatographic, chiroptical and NMR spectroscopic methods. Resolution of reacemic mixtures: Preferential crystallization; Mechanical, chromatographic and kinetic (chemical and enzymatic) resolutions; Diastereoisomer formation: chiral derivatization agents (CDAs), chiral resolving agents (CRAs) and chiral solvating agents (CSAs).

Recommended Books

- 1. E.L. Eliel, S.H. Wilen, M.P. Doyle and P. Michael, *Basic Organic Stereochemistry*, Wiley Interscience, New York (2003).
- 2. P.S. Kalsi. *Stereochemistry and Mechanism Through Solved Problems*, New Age International Publishers, New Delhi, India (2001).
- 3. K. Mislow, Introduction to stereochemistry, W.A. Benjamin, New York, (1966).
- 4. J. Eames and J.M. Peach, *Stereochemistry at a Glance*, Blackwell Publishing (2003).
- 5. D.G. Morris, *Stereochemistry*, Royal Society of Chemistry, U.K (2001).
- 6. M. North, *Principles and Applications of Stereochemistry*, Stanley Thornes: Cheltenham, UK (1998).

CH-430 Retrosynthesis (Cr. 3)

Introduction: retrosynthetic approach and concept of synthons; Functional group interconversions; C-C, C-N, and C-O bond formation. Synthesis of monofunctional target molecules: Alkyl halides, alkenes, alkynes, alcohols, ethers, aromatic compounds, carbonyl compounds, nitrogen compounds, and carboxylic acids and their derivatives. Synthesis of bifunctional target molecules: 1,2-; 1,3-; 1,4-; 1,5-; and 1,6-Difunctionalizations. Cyclizations: Simple intramolecular reactions such as aldol condensation, Claisen condensation and Robinson annulation reactions leading to cyclic structures. Application of the concepts to design the synthesis of various target molecules.

- 1. S. Warren, *Organic Synthesis: The Disconnection Approach*, John Wiley and Sons, Chichester (1992).
- 2. S. Warren, *Workbook for Organic Synthesis: The Disconnection Approach*, John Wiley and Sons, Chichester (1992).
- 3. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, Blackie Academic and Professional, London (1993).

- 4. J. Clayden, N. Greeves, S. Warren and P. Worthers, *Organic Chemistry*, OxfordUniversity (2001).
- 5. C. Willis and M. Willis, Organic Synthesis, Oxford Science Press (1995).
- 6. G.D. Meakins, *Functional Groups: Characteristics and Interconversions*, Oxford Science Press (1996).
- 7. M.B.Smith, *Organic synthesis*, 2nded.,McGraw-Hill,New York (2002)

CH-431 Quantum Organic Chemistry (Cr. 3)

Basic concepts: Wave-particle duality; Properties and nature of wave function; Introduction to the principles of quantum mechanics and their application to chemical systems; Quantum treatment for molecular systems with both electronic and nuclear degrees of freedom; Advance concepts: The Hamiltonian, the Schrodinger equation, the Born-Oppenheimer approximation and Ab initio MOT. Hückel molecular orbital theory (HMOT): Hückel systems; HMO relationship and energy level patterns of linear and cyclic conjugated polyenes; Introduction to density functional theory. Applications of HMO results: HMOT of cyclic and linear π systems; Correlation of HMO results with molecular properties; Prediction and interpretation of IR and UV spectra; Chemical reactivity and reaction mechanism using HMO software.

Recommended Books

- 1. E.V. Anslyn and D.A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books (2004).
- 2. F.L. Ansari, R. Quershi and M.L. Quershi, *Electrocyclic Reactions*, John Wiley & Sons (1999).
- 3. C.M. Quinn, *Computational Quantum Chemistry*, Academic Press (2002).
- 4. K. George, *Introductory Organic Quantum Chemistry*, Academic Press, New York (1962).
- 5. R.A. Jackson, *Mechanism in Organic Reactions*, Royal Society of Chemistry (2004).
- 6. D. Young, *Computational Chemistry: A practical Guide for Applying Techniques* to Real World Problems, Wiley Interscience (2001).
- 7. F. Jonsen, Introduction to Computational Chemistry, John Wiley (1999).
- 8. E. Lewars, *Computational Chemistry*, Kluwer Academic Press (2003).
- 9. C.J. Cremer, Essentials of computational Chemistry, JW. (2004).

CH-432 Spectroscopic Methods in Organic Chemistry-II (Cr. 3)

Nuclear Magnetic Resonance: Theory, Instrumentation and sample handling. ¹H NMR Spectroscopy: Chemical shifts, factors affecting chemical shifts, chemical shifts of organic compounds and their estimation, spin couplings and factors affecting spin couplings, chemical shift equivalence and magnetic equivalence, first order spin systems, double resonance experiments; selective spin decoupling, nuclear overhauser effect and NOE difference spectra. ¹³C NMR Spectroscopy: Differences between ¹H- and ¹³C-NMR spectra, chemical shifts, chemical shifts of organic compounds and their estimation, ¹H BB decoupled and DEPT spectra. Applications: Shift reagents; Dynamic NMR; Stereochemical assignments in different types of compounds; NMR in biochemistry and medicine; NMR spectra of polymers; Structure elucidation of organic compounds by joint applications of UV-visible, IR, NMR and MS.

Recommended Books

- 1. D.L. Pavia, G.M. Lampman and G.S. Kirz, *Introduction to Spectroscopy*, Brooks/Cole Thomson Learning, USA (2001).
- 2. M. Hesse, H. Meier and B. Zeeh, *Spectroscopic Methods in Organic Chemistry*, Georg Thieme Verlag, Stuttgart, Germany (1997).
- 3. R.M. Silverstein, F.X. Webster and D.J. Kiemle, *Spectrometric Identification of Organic Compounds*, John Wiley & sons Inc., USA (2005).
- 4. M. Balci, *Basic*¹*H* and ¹³*C*-*NMR Spectroscopy*, Elsevier (2005).
- 5. E. Breitmaier, *Structure elucidation by NMR in Organic Chemistry a Practical Guide*, John Wiley & Sons, Ltd (2002).
- 6. L.M. Harwood and T.D.W. Claridge, *Introduction to Organic Spectroscopy*, Oxford University Press Inc., New York (1997).
- 7. H. Friebolin, *Basic one-and two-dimensional NMR spectroscopy*, 5th ed., Wiley-VCH, New York (2010).
- 8. Atta-ur-Rahman and M.I. Chaudhary, *Solving Problems with NMR spectroscopy*, Elsevier (1996).
- 9. J.B. Lambert and E.P. Mazzola, *Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods*, Pearson Education (2004).
- 10. R.S. Macomber, A Complete Introduction to Modern NMR Spectroscopy, Johan Wiley & Sons (1998).
- 11. J.K.M. Sanders and B.K. Hunter, *Modern NMR Spectroscopy: a Guide for Chemists*, The University Press, Oxford (1993).
- 12. E. Breitmaier, *Structure Elucidation by NMR in Organic Chemistry: a Practical Guide*, John Wiley, West Sussex (2002).
- 13. M. Younas, Organic Spectroscopy, Ilmi Kitab Khana, Lahore (2004).
- 14. Y.C. Ning, Spectral Identification of Organic Compounds with Spectroscopic Techniques, Wiley-VCH, Weinheim (2005).
- 15. N.E. Jacobsen, NMR Spectroscopy Explained: Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology, John Wiley & Sons (2007).
- 16. E. Pretsch, T. Clerc, J. Seibl, W. Simon and K. Biemann, *Tables of Spectral Data for Structure Determination of Organic Compounds*, Springer (1998).

Pre-requisite: CH-423

Note: In the VII semester the student shall have to take either CH-492 Or CH-498 course, whichever is offered by the department.

CH-492 Organic Chemistry Laboratory-III (Cr. 3)

Multistep synthesis of different types of organic compounds; Purification and identification of synthesized compounds by physical (including UV-visible, IR and MS) and chemical methods; Isolation, purification and identification of some natural products.

Recommended Books

1. B.S. Furniss, Vogel's Textbook of Practical Organic Chemistry Including Qualitative Organic, Longman Group, London (1978).

- 2. H. Becker and I. Hazzard, *Organicum: Practical Handbook of Organic Chemistry*, Reading, Masachuse Addison-Wesley Publishing Co. (1973).
- 3. R. Adams, J.R. Johnson and Wilcox Jr., *Laboratory Experiments in Organic Chemistry*, 6th ed., Collier-M, London (1970).
- 4. A.M. Schoffstall, and B.A. Gaddis, *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, (Druelinger, Melvin L.), McGraw-Hill, Boston (2004).
- 5. J.C. Gilbert, and S.F. Martin, *Experimental Organic Chemistry: a Miniscale and Microscale Approach*, SaundersCollege Publishing, Fort Worth (1998).

Or

CH-498 Thesis/Research Project in Organic Chemistry (Cr. 3)

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

Note: In the VIII semester the student shall have to take either CH-495 Or CH-501 course, whichever is offered by the department.

CH-495 Advanced Organic Chemistry Lab (Cr. 3)

Design, synthesis and characterization of some interesting target molecules.

Or

CH-501 Thesis/Research Project in Organic Chemistry (Cr. 3)

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

Physical Chemistry

CH-441 Polymer Chemistry (Cr. 3)

Introduction: Definition, classification and history. Synthesis: Addition or chain polymerization, "Controlled" free radical polymerization, step-growth polymerization, kinetics of addition and step-growth polymerization, copolymerization. Polymerization processes. Molecular weight of polymers: Distribution, averages, and methods of determination (Viscosity, Osmometry, Light scattering, Size exclusion chromatography). Thermodynamics of polymer solutions and blends: Regular solution theory, the Flory-Huggins theory, solubility parameters, phase behavior of polymer solutions and blends, excluded volume and the Theta temperature. Polymer structure: Introduction to chain isomerism, stereochemistry, configurations, and conformations, polymer crystals, amorphous state of polymers, polymer structure-property relationship. Rheological and mechanical properties: Rheology, typical stress-strain behavior, viscoelasticity, specific physical tests (tensile strength, compressive strength, impact strength, and shear strength).

- 1. Painter P.C. and Coleman M.M., *Fundamental of Polymer Science*, 2nd ed., CRC Press (1997).
- 2. Carraher C.E., *Polymer Chemistry*, 6th ed., Marcel Dekker (2003).

- 3. Young R.J., *Introduction to Polymers*, Chapman and Hall Ltd. (1981).
- 4. Stevens M.P., *Polymer Chemistry: An Introduction*, OxfordUniversity Press (1999).
- 5. Sperling L.H., *Introduction to Physical Polymer Science*, 4th ed., Wiley Interscience (2006).

CH-442 Molecular Spectroscopy (Cr. 3)

Introduction: Interaction of electromagnetic radiation with matter, symmetry properties of molecules, classification of spectroscopy, factors affecting the width and intensity of spectral transitions, applications. Rotational spectroscopy: Introduction, rotational spectroscopy of various classes of molecules including diatomic rigid rotator (assuming a rigid rotator model) and non-rigid molecules, polyatomic linear molecules, and symmetric tops, the stark effect, applications of rotational spectroscopy. Vibrational spectroscopy: The vibrating diatomic molecules as simple harmonic oscillator model, the anharmonic diatomic oscillator, diatomic vibrating-rotator, the interaction of rotations and vibrations (breakdown of the Born-Oppenheimer approximation), polyatomic molecules, normal modes of vibrations, linear and symmetric top type polyatomic vibrators, applications of vibrational spectroscopy of diatomic molecules: rotational fine and vibrational coarse structures, the Frank-Condon principle, dissociation, interpretation of spectra-a few case studies, fluorescence and phosphorescence. Nuclear magnetic resonance spectroscopy: Principles and applications, interpretation of spectra-a few case studies.

Recommended Books

- 1. C.N. Banwell, *Fundamentals of Molecular Spectroscopy*, 3rd ed., McGraw-Hill, UK (1983).
- 2. G.M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill (International Student Edition) (1990).
- 3. G. Aruldhas, *Molecular Structure and Spectroscopy*, Prentice-Hall (India) (2004).
- 4. I. N. Levine, *Physical Chemistry*,6th ed., McGraw Hill Higher Education (2009).
- 5. J.M. Hollas, *Modern Spectroscopy*, 4th ed., Wiley (2004).

CH-443 Chemical Kinetics (Cr. 3)

Rate: Review of essentials of rate laws and order of reactions, 3rd order reaction differential and integrated rate equations. Reaction mechanisms; mechanistic interpretation of rate laws, equivalent kinetic expressions. Reaction rate Theories: Kinetic Theories of chemical reactions: Collision theory, Transition state theory (TST), models based upon thermodynamics, statistical mechanics and quantum mechanics, Applications of TST; temperature effects; heat capacity of activation; composite rate constants; pressure effects and volume of activation; interpretation of activation parameters. Composite reactions: reversible 1st and higher order reactions, parallel and concurrent reactions, consecutive first order reactions; steady state approximation; rate controlling step; kinetics of polymerization; catalyzed reactions; characteristics of chain reactions; flow methods for rapid reactions, shock wave methods, chemical relaxation methods, quenching by florescence method, flash and laser photolysis, pico-second and femto-second methods and pulse radiolysis.

- 1. I.N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).
- 2. K.J. Laidler, *Chemical Kinetics*, 3rd ed., Pearson Education Ins., Singapore, (1987).
- 3. An Introduction to Chemical Kinetics, Michel Soustelle, Wiley-ISTE.(2011).
- 4. J.H. Espenson, *Chemical Kinetics and Reaction Mechanisms*, 2nd ed., McGraw HillSingapore (1995).
- 5. P.L. Houston, *Chemical Kinetics and Reaction Dynamics*, Dover edition, New York, November 17, 2006.
- 6. A.A.M. Frost and R.G. Pearson, *Kinetics and Mechanism*, 3rd ed., Butterworths, London (1969).

CH-444 Solid State Chemistry (Cr. 3)

Fundamentals: Unit cells and crystal systems. Lattices and their description: Bravais lattice; Miller indices; unit cell contents. Point groups and their relevant classification based on symmetry. Space groups and crystal structures: Closed packed structures (cubic, hexagonal, tetragonal and other packing arrangements). Important structure types (Rutile, Rock Salt, Zinc Blende, Wurtzite. etc). Perfect and imperfect crystals; types of defects with description. Diffusion of ions in solids; dislocation; mechanical properties and reactivity of solids. Structure and surface analysis: XRD- patterns for crystalline, semicrystalline and amorphous materials, Debye Sherrer formula and crystallite size, difference between crystallite and particles, surface morphology. Theories of electrical conductance in different types of solids.

Recommended Books

- 1. A.R. West, *SolidState Chemistry and its Applications*, 2nded., Wiley (2013).
- 2. W.D. Callister, *Material Science and Engineering*, 6th ed., John Wiley, New York (2003).
- 3. D.W. Bruce, D. O'Hare and R.I. Walton (Editors), *Structure from Diffraction Methods: Inorganic Materials Series*, Wiley (2014).
- 4. R.J.D. Tilley, Understanding Solids: The Science of Materials, 2nded., Wiley (2013).

CH-445 Electrochemistry (Cr. 3)

Overview of basic concepts; Types of electrodes, electrochemical cells, electrochemical series, applications of electrode potential. Theories of electrolytes; interfacial phenomenon, electrical double layer, Göuy, Stern, Helmholtz models. Electrode kinetics: difference between controlled potential and controlled current techniques, essentials of heterogeneous kinetics, Butter-Volmer equation, over potential, zero, low and high field approximations, symmetry parameter, concept and use of exchange current, Tafel equation and Tafel plots. Polarography and voltammetry: cyclic voltammetry concept of anodic and cathodic current, peak potential, half wave potential, reversibility criteria. Batteries and fuel cells: working principle, structural components, types of batteries, concept of primary and secondary batteries, examples of fuel cell.

- 1. A.J. Bard and L.R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd ed., Wiley (2001).
- 2. J. Wang, *Analytical Electrochemistry*, 3rd ed., Wiley-VCH, New Jercy (2006).
- 3. V.S. Bagotskii, Fundamentals of Electrochemistry, 2nd ed., Wiley, New Jercy

(2005).

- 4. P.H. Rieger, *Electrochemistry*, 2nd ed., Chapman and Hall, New York (1993).
- 5. D. Pletcher and H. Saxton, A First Course in Electrode Processes, 2nd ed., RSC publications, UK (2009)
- 6. J.O'M. Bockris, A.K.N. Reddy and M.F. Gomboa, *Modern Electrochemistry: Fundamentals of Electrodes*, 2nd ed., Springer (2000).

CH-446 Nuclear and Radiation Chemistry (Cr.3)

Fundamental: Brief history of discovery of various nuclear and sub-nuclear particles. Nuclear liquid drop model, shell model; Nuclear composition, nuclear size and density, isotope chart, classification of nuclides on the basis of composition, stability, binding energy, nuclear mass defect and binding energy, various nuclear characteristics including half-life, decay constant, decay energy. Nuclear decay processes including: α -decay, β -decay, positron emission, electron capture. Nuclear kinetics: Equations of decay and growth processes for successive and branched decay, Natural and artificial decay series and applications, transient and secular equilibria. Radiation chemistry: Basic types of nuclear radiations, Interaction of radiation with matter. Introduction to dosimetry; Applications: Medical and industrial applications of nuclear and radiation chemistry.

Recommended Books

- 1. W.D. Loveland, D.J. Morrissey and G.T. Seaborg, *ModernNuclear Chemistry*, John Wiley & Sons, New York (2006).
- 2. G.R. Choppin, J.O. Liljenzin, J. Rydberg and C. Ekberg, Revised Ed., *Radiochemistry and Nuclear Chemistry*, Academic Press, USA (2013).
- 3. H.J. Arnikar, *Essentials of Nuclear Chemistry*, New Age International publishers Ltd., Wiley Eastern Ltd., New Delhi (1995).
- 4. G. Friedlander and W Kennedy, *Nuclear and Radiochemistry*, John Wiley & Sons, New York (1981).
- 5. K.H. Lieser, *Nuclear and Radiochemistry (Fundamentals and Applications)*, John Wiley-VCH Weinheim (2001).

CH-447 Surface Chemistry (Cr. 3)

Adsorption: Surface and interface, interfacial tension, adsorption forces, thermodynamics of adsorption, porosity, particle size distribution, physisorption and chemisorptions. Adsorption isotherms: Freundlich, Langmuir, BET, Gibbs, force field in fine pores, microporosity. The use of gas adsorption for the determination of surface area and pore size distribution. Catalysis: homogeneous and heterogeneous catalysis and gas-solid interface, enzyme catalysis, gas reactions at solid surfaces, diffusion limitations and compensation effect. Chemisorption at metal and oxide surfaces, catalysis for industrial processes; catalytic reactors, supported metal catalysts, catalysis in atmospheric pollution control.

- 1. G.C. Bond, *Heterogeneous Catalysis: Principles and Applications*, 2nd ed., Clarendon Press, Oxford (1987).
- 2. S.J. Gregg and K.S.W. Sing, *Adsorption, Surface area and Porosity*, 2nd ed., Academic press, INC, London Ltd. (1982).
- 3. A.W Adamson and A.P. Gast, *Physical Chemistry of Surfaces*, 6th ed., John Wiley

and Sons, Inc New York (1997).

- 4. D.F. Evans and H. Wennerström, *The Colloidal Domain Where Physics, Chemistry, Biology and Technology Meet*, VCH Publishers, Inc., New York (1994).
- 5. R.M. Pashley and M.E. karaman, *Applied Colloid and Surface Chemistry*, John Wiley and Sons Ltd., (2004) ISBN: 0470868821 (HB).

CH-448 Photochemistry (Cr.3)

Fundamentals: Light and nature of electromagnetic radiations, electronic structure of atoms, interaction of light with atoms and molecules, term symbols, absorption and emission of radiations. Fluorescence, phosphorescence, Jablonski diagram, chemiluminescence, quantum yields of photochemical reactions, actinometry, kinetics of photochemical reactions. Laws of photochemistry: Photo excited molecules, monophotonic and multiphotonic processes, photodissociation. Photo-electrochemistry, photochemical reactions in gas phase and in solutions, photophysics and photochemistry of metal complexes. Applied Photochemistry: Photography, Photo-imaging, photochromism, vision, photochemistry of polymers, solar energy storage, photochemistry in synthesis, optical brighteners and photo-medicine.

Recommended Books

- 1. P. Suppan, *Chemistry and Light*, The Royal Society of Chemistry, London (1994).
- 2. R.P. Wayne, *Principles and Applications of Photochemistry*, OxfordUniversity Press (1988).
- 3. Wayne and Richard P.,*Photochemistry*, Macmillan (1988).
- 4. J.G. Calvert, and J.N. Pitts, *Photochemistry*, John Wiley and Sons Inc., New York (1966).
- 5. C.E. Wayne, *Photochemistry*, OxfordUniversity Press, London (1996).
- 6. M. Bhaskaram, S. Sriram and K. Iniewski, *Energy Harvesting with Functional Materials and Microsystems*, CRC Publisher, Taylor and Francis group, UK (2014).
- 7. J. N. Pitts, G. S. Hammond, K. Gollnick. Advances in Photochemistry, Volume 12, John Wiley & Sons (2009).

CH-449 Thermodynamics (Cr. 3)

Basic concepts: State and path functions and their discrimination by Euler's theorem, Thermodynamic processes, Heat capacities, Chemical potential, Enthalpy and entropy and their dependence on volume (Joule-Thomson effect) Joule-Thomson coefficient and its determination, Free energy change, Relation between thermodynamic functions, Laws of thermodynamics, Zeroth, 1st, 2nd and 3rd laws of thermodynamics, Applications of 1st and 2nd laws of thermodynamics. Equilibrium thermodynamics: Relation of entropy and energy with equilibrium constant, and their dependence on temperature, Van't Hoff's equation, Clausius-Clapeyron equation. Phase rule: Phase equilibrium, phase diagrams of one component system and multicomponent systems, cooling curves.

Recommended Books

1. P.A. Peter, *Chemical Thermodynamics*, OxfordUniversity Press (1983).

- 2. I.M. Klotz and R.M. Rosenberg, *Chemical Thermodynamics: Basic Concepts and Methods*, 7th ed., Wiley Backwell (2008).
- 3. D.A. McQuarrie and J.D. Simon, *Molecular Thermodynamics*, University Science Books, U.S. (2004).
- 4. S.E. Brain, *Basic Chemical Thermodynamics*, 5th ed., ImperialCollege Press (2004).

CH-450 Solution Chemistry (Cr. 3)

Fundamentals of solutions: concept of solute and solvent, mixtures and their importance. Classification of solutions, concentration units and their interconversion, activity and activity coefficients, distillation and concept of azeotropic mixture, interactions in solutions; solvent-solvent interactions, solute-solvent interactions, ion-ion interactions, ion-pairing, structure of solvates. Measurements: Microscopic and macroscopic properties. Colligative properties; Lowering of vapor pressure, elevation of boiling point, depression of freezing point, elevation of osmotic pressure and experimental methods for the determination of these properties, partial molar quantities, solvation number of metal ions and its determination.

Recommended Books

- 1. J. Burgess, *Ions in Solution: Basic Principles of Chemical Interactions*, Ellis Harwood Ltd. UK (1999).
- 2. C. Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, 3rd ed., VCH, Weinheim, Germany (2003).
- 3. I.N. Levine, *Physical Chemistry*, 6th ed., Tata McGraw-Hill (2008).

CH-451 Colloids and Surfactants (Cr. 3)

Introduction: Capillarity; Surface tension, Young-Laplace and Kelvin equations, orientation at interfaces, thermodynamics of binary systems, the Langmuir and Gibbs adsorption equations, Self assembled monolayer and its characterization. Surfactants: Nature and classification, micellization, solubilization, factors affecting self aggregation, determination of critical micelle concentration and evaluation of thermodynamic parameters of micellization, micellar catalysis and inhibition. Emulsion: Emulsion stability, aging and inversion of emulsions, hydrophile-lipophile balance, microemulsions, wetting and contact angle. Colloidal solutions: Rheology of dispersions, static and dynamic light-scattering, lyophobic and association colloids, forces in colloidal systems.

Recommended Books

- 1. A.W. Adamson, *Physical Chemistry of Surfaces*, 5th ed. Wiley-Interscience Publication, John Wiley & Sons, Inc., New York (1990).
- 2. P.C. Hiemenz and Rajagopalan, *Principles of Colloid & Surface Chemistry*, 3rd ed., Marcel Dekker Inc., New York (1997).
- 3. M.J. Rosen, *Surfactants and Interfacial Phenomena*, 4thed., Wiley-Interscience Publication, John Wiley & Sons, New York (2012).

CH-452 Quantum Chemistry (Cr. 3)

Quantum mechanics and its significance in chemistry, quantization, postulates, operators, Hermitian operators, differential equations and their solutions, particle in a rectangular well and energy levels, Schrödinger's equation of free particle (allowed, forbidden and possible energy levels), harmonic and anharmonic oscillators, vibrations of molecules, angular momentum, rotation of a particle in a plane and on a sphere, rotational motion of molecules, real chemical systems such as hydrogen atom and hydrogen like atoms. Multielectron atoms: Approximate methods, Perturbation method, variation principle, Pauli principle, Hund's rule, spin-orbit interaction. Quantum treatment of molecules:Valence bond and molecular orbital theories, HMO theory and pi-electron calculations, band gap theory and semiconductors.

Recommended Books

- 1. D.F. Micheal, *Elements of Quantum Mechanics*, OxfordUniversity Press (2005).
- 2. D.O. Hayward, *Quantum Mechanics for Chemists*, 1st ed., John Wiley (2003).
- 3. D.A. McQuarie, *Quantum Chemistry*, OxfordUniversity Press, Oxford, UK, (1983).
- 4. I.N. Levine, *Quantum Chemistry*, 6th. ed., Prentice Hall London (2010).

CH-453 Numerical Methods and Computational Chemistry (Cr. 3)

Basic operation of computer, hardware, software. Packages useful in chemistry, experimental data manipulation and calculations. Computer aided numerical methods: Least square curve fitting method for linear, quadratic, cubic, exponential and logarithmic and other functions; statistical analysis. Numerical differentiation. Numerical integration: Rectangular, trapezoidal and parabolic methods of approximation. Molecular modeling: Mechanical models, model building using different force field parameters, energy calculations, geometry optimization, potential energy surfaces. Prediction of various properties.

Recommended Books

- 1. K. Smith, *Calculus with Applications*, Brooks/Cole, Pacific Grove (1998).
- 2. R. Kumari, *Computers and Their Applications to Chemistry*, Narose Publishing House, New Delhi, India (2005).
- 3. R.J. Mortimer, *Mathematics for Physical Chemistry*, 3rd ed., Elsevier Academic Press (2005).

CH-454 Statistical Mechanics (Cr. 3)

Introduction: Permutation and combination. Description of various systems, Concepts of states, accessible states and distribution of energy, probability concepts. Microstates and Macrostates. Maxwell-Boltzmann's statistics for the systems of independent particles. The Bose-Einstein's statistic, Fermi-Dirac's statistics, statistical interpretation of entropy. Maxwell-Boltzmann's distribution function, Bose-Einstein's distribution function and Fermi-Dirac's distribution function. Comparison for distribution functions for indistinguishable particles. Statistical Themodynamics: Partition functions, relationship of partition functions to various thermodynamic functions, monatomoc ideal gas. Quantized linear oscillator. Specific heat capacity of a diatomic gas. Translational partition function, vibrational partition function and rotational partition function. Application of partition functions to calculate equilibrium constant.

- 1. L.K. Nash, *Element of Classical and Statistical Thermodynamics*, Adison-Wesley Publishing company, Inc, (1968).
- 2. F.W. Sears and G.L. Sakinger, *Thermodynamics Kinetic Theory, and Statistical Thermodynamics*, 3rd ed., Adison-Wesley Publishing company, Inc. (1975).

- 3. E.B. Smith, *Basic Chemical Thermodynamics*, 4th ed., OxfordUniversity Press (1990).
- 4. J.M. Seddon and J.D. Gale, *Thermodynamics and Statistical Mechanics*, Royal Soc. Chem., UK (2002).
- 5. J.G. Aston and J.J. Fritz, *Thermodynamics and Statistical Thermodynamics*, John-Wiley, New York (1987).
- 6. E. Thomas and P. Reid, *Thermodynamics, Statistical Thermodynamic and Kinetics*,1st ed., Benjamin Cummings (2006).

Note: In the VII semester the student shall have to take either CH-493 Or CH-499 course, whichever is offered by the department.

CH-493 Physical Chemistry Lab-III (Cr. 3)

Note: The students are required to perform at least ten experiments.

- 1. Investigation of conductivity of different electrolyte solutions in various media.
- 2. Determination of partial molar volumes and excess molar volumes for binary and ternary systems.
- 3. Polarimetric determination of specific rate constant for inversion of sucrose and determination of activation energy.
- 4. Determination of the composition of complex ion in solution by spectrophotometric method (Job's method) for the systems Fe³⁺-salicyclic acid, Ni²⁺-ethyldiamine.
- 5. Effect of mixture composition on the proton NMR spectrum of protic system, investigation of intermolecular interactions.
- 6. Voltammetric investigations of given compound(s) under variable experimental conditions.
- 7. Effect of controlled heating on the composition of given solids and monitoring of their IR-spectra.
- 8. Purification of the given commercial solvent using pertinent methods of separation (distillation, fractional distillation, reflux).
- 9. Average molar mass determination of a given polymer by viscosity measurement.
- 10. Determination of conductivity of given electrolytes at infinite dilution at different temperatures and their correlation with the viscosities of medium.
- 11. Determination of activation energy for the base catalyzed hydrolysis of the given ester and investigation of reaction mechanism at different temperatures.
- 12. Study of two phases by mixing water and 1-butanol by refractometer.
- 13. Spectroscopic investigation of the distribution of a given transition metal ion between the two phases.
- 14. Determination of rate of oxidation of benzyl alcohol in acid permanganate by spectrophotometric method.
- 15. Determination of chain flexibility of polystyrene in different solvents.
- 16. Determination of critical micelle concentration and thermodynamic parameters of block polymers.

Recommended Books

1. A.M. Halpern and G.C. Mcbane, *Experimental Physical Chemistry: A Laboratory Textbook*, W.H. Freeman (2006).

- 2. C. Garland, J. Nibler, D. Shoemaker, *Experiments in Physical Chemistry*, 8th Edition, McGraw Hill Higher Education (2008).
- 3. J.A. Beran, *Chemistry in the Laboratory: A Study of Chemical and Physical Changes*, Halsted Pr Publishers (1996).

Or

CH-499 Thesis/Research Project in Physical Chemistry (Cr. 3)

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

Note: In the VIII semester the student shall have to take either CH-496 Or CH-502 course, whichever is offered by the department.

CH-496 Advanced Physical Chemistry Lab-IV (Cr. 3)

The course teacher(s) shall offer advanced level practicals involving different experimental facilities available in the section/department. The details of the laboratory work and the equipment involved shall be decided by the teacher concerned on the basis of the courses taught.

Or

CH-502 Thesis/Research Project in Physical Chemistry (Cr. 3)

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.
