SYLLABUS

FOR

MASTERS PROGRAMME (M.Sc.)

IN

CHEMISTRY

(BATCH-2016 and BATCH-2017)

UNDER

CHOICE BASED CREDIT SYSTEM

(CBCS)

DEPARTMENT OF CHEMISTRY

ISLAMIC UNIVERSITY OF SCIENCE AND TECHNOLOGY,

AWANTIPORA, PULWAMA, KASHMIR, J&K, INDIA, 192122.

Department of Chemistry
Islamic University of Science and Technology

Master's Programme

A Master's Programme consists of a set of Core Courses and Optional Course. The entire course carries choice based credit system. A Master's degree in Chemistry course is divided in to 04 semesters comprising 02 odd semesters and 02 even semesters.

Credits

The term credit is used to describe the quantum of syllabus for various programmes in terms and hours of study. It indicates differential weightage given according to the contents and duration of the courses in the curriculum design.

Courses

Each course may consist of Lectures/ Tutorials/ Laboratory work/ Seminar/ Project work/ Practical training report/ Viva voce etc.

Subject Code Fixation

The following code system (5 characters) is adopted for Post graduate course in chemistry

PXX PG code for department

X Course Type

X Specification of that course

Example **PCH** **CC** **101** → **PCH-CC-101**

PG Code Core Course Specification of that course

CC– Core Courses: Theory & Practical

DCE – Discipline Centric

OE-Open Electives

Department of Chemistry
Islamic University of Science and Technology

Total Credit and Marks Distribution for the Four Semesters

Course Type	No of Papers	Credits per Paper	Total Credits	Marks per Paper	Total Marks
Core Course (Theory)	14	4	56	100	1400
Core Course (Practical)	5	2	10	100	500
Project Core	1	4	4	100	100
Discipline Centric Elective (DCE)	6	3	18	100	600
Open Elective (OE)	2	2	4	50	100
Total	28		92		2700

Department of Chemistry
Islamic University of Science and Technology

Overview of the Course Scheme of Department of Chemistry based on Choice based Credit System for First Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
I	PCH-CC-101	Metal Complexes and Reaction Mechanism	CC	30	70	100	3	1	0	4	24
	PCH-CC-102	Stereochemistry and Reaction Intermediates	CC	30	70	100	3	1	0	4	
	PCH-CC-103	Chemical Kinetics and Quantum Chemistry	CC	30	70	100	3	1	0	4	
	PCH-DCE-104	Introduction to Spectroscopic Methods	DCE	30	70	100	3	0	0	3	
	PCH-DCE-105	Mathematics for Chemists	DCE	30	70	100	3	0	0	3	
	PCH-DCE-106	Green Chemistry	DCE	30	70	100	3	0	0	3	
	PCH-CC-107	Laboratory Course in Physical Chemistry	CC	30	70	100	0	0	2	2	
	PCH-CC-108	Laboratory Course in Inorganic Chemistry	CC	30	70	100	0	0	2	2	
		Chosen from the list of open elective courses	OE	15	35	50	2	0	0	2	

CC = Core Course
DCE = Discipline Centric
OE = Open Elective Course

A total of 24 credits to be taken by students with following breakup:
CC = 16 Credits
DCE = 6 Credits
OE = 2 Credits

Open elective course offered by the Department of Chemistry for other Departments of the University.

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
1st	PCH-OE-101	Biomolecules	OE	15	35	50	2	0	0	2	2

Department of Chemistry
Islamic University of Science and Technology

Overview of the Course Scheme of Department of Chemistry based on Choice based Credit System for Second Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
II	**PCH-CC-201**	Metal Clusters and Electronic Spectra of Metal Complexes	CC	30	70	100	3	1	0	4	24
	PCH-CC-202	Mechanism of Organic Reactions	CC	30	70	100	3	1	0	4	
	PCH-CC-203	Quantum Chemistry & Electrochemistry	CC	30	70	100	3	1	0	4	
	PCH-DCE-204	Chromatographic Techniques	DCE	30	70	100	3	0	0	3	
	PCH-DCE-205	Bioinorganic Chemistry	DCE	30	70	100	3	0	0	3	
	PCH-DCE-206	Conducting Polymers	DCE	30	70	100	3	0	0	3	
	PCH-CC-207	Laboratory Course in Organic Chemistry	CC	30	70	100	0	0	2	2	
	PCH-CC-208	Laboratory Course in Analytical Chemistry	CC	30	70	100	0	0	2	2	
		Chosen from the list of open elective courses	OE	15	35	50	2	0	0	2	

CC = Core Course
DCE = Discipline Centric
OE = Open Elective Course

A total of 24 credits to be taken by students with following breakup:
CC = 16 Credits
DCE = 6 Credits
OE = 2 Credits

Open elective course offered by the Department of Chemistry for other Departments of the University.

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
2nd	PCH-OE-201	Introduction to Nanotechnology	OE	15	35	50	2	0	0	2	2

Department of Chemistry
Islamic University of Science and Technology

Overview of the Course Scheme of Department of Chemistry based on Choice based Credit System for Third Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
III	PCH-CC-301	Organometallic Chemistry	CC	30	70	100	3	1	0	4	24
	PCH-CC-302	Pericylclic Reactions and Organo-Photochemistry	CC	30	70	100	3	0	0	3	
	PCH-CC-303	Thermodynamics and Solid-State Chemistry	CC	30	70	100	3	1	0	4	
	PCH-CC-304	Polymers and Nanotechnology	CC	30	70	100	3	0	0	3	
	PCH-DCE-305	Spectroscopy of Organic Compounds	DCE	30	70	100	3	0	0	3	
	PCH-DCE-306	Inorganic Spectroscopy	DCE	30	70	100	3	0	0	3	
	PCH-DCE-307	Chemo-informatics	DCE	30	70	100	3	0	0	3	
	PCH-CC-308	Advance Laboratory Course	CC	30	70	100			4	4	

CC = Core Course
DCE = Discipline Centric

A total of 24 credits to be taken by students with following breakup:
CC = 18 Credits
DCE = 6 Credit

Open elective course offered by the Department of Chemistry for other Departments of the University.

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
3rd	PCH-OE-301	Drugs and Chemotherapy	OE	15	35	50	2	0	0	2	2

Department of Chemistry
Islamic University of Science and Technology

Overview of the Course Scheme of Department of Chemistry based on Choice based Credit System for Fourth Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
IV	PCH-CC-401	Natural Product and Medicinal Chemistry	CC	30	70	100	3	1	0	4	20
	PCH-CC-402	Statistical Thermodynamics and Colloidal Chemistry	CC	30	70	100	3	1	0	4	
	PCH-CC-403	Retro-synthesis and Heterocyclic Chemistry	CC	30	70	100	3	1	0	4	
	PCH-CC-404	Group theory and Analytical Techniques	CC	30	70	100	3	1	0	4	
	PCH-CC-405 **Project and Dissertation**					100				4	

CC = Core Course
DCE = Discipline Centric

A total of 20 credits to be taken by students

Open elective course offered by the Department of Chemistry for other Departments of the University.

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credit	Total Credit
				Internal	Final	Total	L	T	P		
4th	PCH-OE-401	Surfactants, Soaps, and Detergents	OE	15	35	50	2	0	0	2	2

Semester-I

M.Sc. FIRST YEAR
First Semester
Core Course
Course Title: Metal-Complexes and Reaction Mechanism
Course Code: PCH-CC-101

Credits = 4
M.M. = 100 (70+30)

Unit-I: Metal-Ligand Bonding

Crystal field theory (CFT), Salient features, Spectrochemical series, Splitting of d-orbitals in octahedral and tetrahedral geometry, Applications of CFT: Colours of transition metal complexes, Magnetic properties of octahedral complexes, Jahn-Tellar distortion, Factors affecting CFSE, Limitations of CFT, Experimental evidence for metal-ligand covalent bonding in complexes, Nephelauxetic effect, Ligand field theory,
M.O. Theory, π-bonding and M.O. theory in octahedral, Tetrahedral and square-planar complexes.

Unit-II: Stability of Transition Metal Complexes

Step-wise and Overall formation constant and their relationship, Trends in step-wise constant (kinetic and thermodynamic stability) of metal complexes, Factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, Chelate effect, Macrocyclic effect, their thermodynamic origin, Crown ether complexes and cryptands. Determination of binary formation constant by pH metry and spectrophotometry.

Unit-III: Reaction Mechanism in Octahedral Transition Metal Complexes

Reactivity of metal complexes, Inert and labile complexes, Kinetic application of valence bond and crystal field theories, Kinetics of octahedral substitution, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, Anation reactions, reactions without metal ligand bond cleavage.

Unit-IV: Reaction Mechanism in Square Planar Complexes

Substitution reactions in square planar complexes, Trans-effect, Mechanism of substitution reaction. Redox reactions, Electron transfer reactions, Mechanism of one electron transfer reaction, Outer-Sphere Reactions, Cross Reactions and marcus-hush theory, Inner-sphere reactions.

Books Recommended:

1. Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4th Edn. 2008.
2. Reaction Mechanism of Inorganic and Organometallic Systems; R. B. Jordan; Oxford; 3rd Edn.; 2007.
3. Comprehensive Coordination Chemistry eds., G. Wilkinson, R. D. Gillars and J. A. Mc Clevert, Pergamon. 2nd Edn. 2003.
4. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley 6th Edn, 1999.
5. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon. 2nd Edn, 1997.
6. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier. 2nd Edn, 1997.
7. Inorganic and Organometallic Reaction Mechanisms; 2nd edn.; Jim D. Atwood; Wiley; 1997
8. Mechanisms of Inorganic Reactions; D. Katakis, G. Gordon; Wiley; 1987.
9. Magnetochemsitry, R. L. Carlin, Springer Verlag, 1986.
10. Inorganic Chemistry; K. F. Purcell, L. C. Kotz; Saunders; 1977.
11. Electronic Spectra of Transition Metal Complexes; D. Sutton; McGraw Hill; 1968.
12. Mechanisms of Inorganic Reactions; F. Basolo, R.G. Pearson; Wiley; 2nd Edn.; 1967.

M.Sc. FIRST YEAR
First Semester
Core Course
Course Title: Stereochemistry and Reaction Intermediates
Course Code: PCH-CC-102

Credits = 4
M.M = 100 (70+30)

Unit-I: Nature of Bonding in Organic Molecules

General overview of bonding in organic compounds. Alternant and non-alternant hydrocarbons. Conjugation and cross-cojugation, Aromaticity in benzenoid and non-benzenoid compounds, Huckel's rule of aromaticity, Annulenes, Antiaromaticity, Homoaromaticity, PMO approach., Inclusion compounds-cyclodextrins, Catenanes and rotaxanes, Fullerenes.

Unit-II: Stereochemistry

Optical activity and chirality, Molecules with more than one chiral center, Erythro- and threo isomers, Asymmetric synthesis. Methods of resolution, Optical purity, Cram's rule. Fischer's projection formula. Absolute configuration- R, S notation of biphenyls and allenes. Study of dissymmetry of allenes, Biphenyls, Spiro compounds, Trans-cyclooctene and cyclononene. Chirality due to helical shape. Enantiotopic and diastereotopic atoms, Groups and faces, Stereochemistry of the compounds containing nitrogen and sulfur.

Unit-III: Conformational Analysis

Conformational analysis of mono, di and tri-substituted cyclohexanes and their stereochemical features (geometrical and optical isomerism), Conformation and reactivity of substituted cyclohexanes, cyclohexanol (Oxidation and Acylation) and cyclohexanone (Reduction). Conformation and stereochemistry of cis and trans-decalin and 9-methyldecalin, Interconversion of sawhorse, Newman and fischer projections.

Unit-IV: Reactive Intermediates

Carbocations: Generation, Structure and stability, Classical and non-classical, Neighbouring-group participation (NGP), Ion pairs, Molecular rearrangement in acyclic, monocyclic and bicyclic systems, Stability and reactivity of bridge-head carbocations.
Carbanions: Generation, structure and stability, Amident ions and their general reactions.
Radical: Generation, structure, stability and reactions, Cage-effects, Radical–cations and radical-anions.
Carbenes: Formation and structure, Reactions involving carbenes and carbenoids.
Nitrenes: Generation, Structure and reactions of nitrenes.
Arynes: General methods of generation and reactivity.
Singlet oxygen: Generation and reactions with organic substrates.

Books Recommended:

1. Advanced Organic Chemistry, Reactions, Mechanism and Structure, Jerry March, John Wiley. 7th Edn.; 2013
2. Stereochemistry of Organic Compounds, D. Nasipuri. 3rd Edn. 2011
3. Advanced Organic Chemistry, J. Singh and L. D. S. Yadav, Pragati Prakashan. Meerut India, Ed., 2011.
4. Advanced Organic Chemistry; F. A. Carey and R. J. Sundberg; Springer Plenum; 5th Edn.; 2007.
5. Organic Chemistry by I. L. Finar Vol-I and II,. ELBS Publications. 6th Edn.; 2002.
6. A Guide Book to Mechanism in Organic Chemistry; Peter Sykes; Longman; 6th Edn.; 1996
7. Organic Chemistry, R. T. Morison & R. N Boyd, Prentice Hall, 6th Edn.; 1992.
8. Carbenes, Nitrenes and Arynes, T. L. Gilchrist and C. W. Rees, Thomas Nelson and Sons Ltd., London. 1971.

M.Sc. FIRST YEAR
First Semester
Core Course
Course Title: Chemical Kinetics and Quantum Chemistry
Course Code: PCH-CC-103

Credits = 4
M.M. = 100 (70+30)

Unit-III: Chemical Kinetics-I

Kinetic analysis of experimental dat**a:** Estimation of order and rate constant from concentration-time data (Differential rate method and Integral rate method).
Fast reactions: General features of fast reactions, Study of fast reactions by flow method, Relaxation method and flash photolysis.
Theories of chemical reactions: Activated complex theory of reaction rates, Statistical & thermodynamic formulations, Comparison with collision theory.
Theories of unimolecular reactions (Lindman, Hinshelwood theories), Potential energy surfaces.

Unit-IV: Chemical Kinetics –II

Surface Reactions: Unimolecular& bimolecular surface reactions, Langmuir-Hinshelwood & Langnuir-Riedel mechanism, Classical & Statistical treatments.
Reactions in liquid solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic reactions: Single & double sphere models of ionic reactions, Hammett equation, Catalysis: introduction to catalysis, Mechanism of catalysis, Use of solvents as catalysts, Enzyme catalysis, Michaelis–Menten Equation, Inhibition of enzymes, Effects of pH, Temperature effects.

Unit-III: Quantum Chemistry-I

Operator concept, Quantum mechanical operators (cartesian and spherical polar co-ordinate systems), Schrodinger equation (Time dependent and independent), Properties of quantum mechanical operators, Postulates of quantum mechanics.
Particle in a box problem, The solution of problems of harmonic oscillator & the rigid rotator.

Unit-IV: Quantum Chemistry-II

Born-Oppenheimer approximation, Solution of the Hydrogen-like atom problem- radial and angular wave functions. Angular momentum and electronic structure of atom, General theory of angular momentum, Eigen functions and eigenvalues of angular momentum operators, Ladder operators, Spin angular momentum, Anti-symmetry and Pauli's principle, Wave functions of poly-electron atoms, Slater determinant, Atomic term symbols, Term separation of p^n and d^n configurations, Spin-Orbit coupling, Zeeman splitting.

Books Recommended:

1. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill, 4th Edn.; Revised, 2002.
2. Chemical Kinetics and Catalysis, R. I. Masel, Wiley, 2001.
3. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W. L. Hase, 2nd Edn.; 1998.
4. Introductory Quantum chemistry- A. K. Chandra, Tata McGraw Hill, 1998.
5. Methods of Molecular Quantum Mechanics, R. Mc Weeny, Academic Press, 2nd Edn.; 1992.
6. Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7th Edn.; 2013.
7. Quantum Chemistry, Prasad, New Age Publishers, 4th Edn.; 2010.

M.Sc. FIRST YEAR
First Semester
Discipline Centric
Course Title: Introduction to Spectroscopic Methods
Course Code: PCH-DCE-104

Credits = 3
M.M = 100 (70+30)

Unit-I: Statistical Analysis and Validation

General introduction: Instrumental and non-Instrumental methods of analysis in analytical chemistry. Errors in chemical analysis, Classification of errors, Determinate and indeterminate errors, Accuracy and precision, Mean, Median, Average deviation and standard deviation, Confidence limit, Correlation coefficient and regression analysis, Comparison of methods: F-test and T-test, Rejection of data based on Q-test, Least squares method for deriving calibration graph, Concepts and difference between sensitivity, (LOD) and (LOQ).

Unit-II: Microwave and IR Spectroscopy

General introduction to spectroscopy, Principle of microwave spectroscopy, Classification of molecules, Rigid-rotor model, Effect of isotopic substitution on the transition frequencies, Intensities, non-rigid rotor, Stark effect and applications, Principle of IR, Modes of vibration in molecules, Energy, Force constant and bond strength, Anharmonicity, Morse Potential energy diagram, Derivation of selection rules for diatomic molecules based on harmonic oscillator approximation, Characteristic vibrational frequencies of various functional groups, Effects of hydrogen bonding and Solvent effect on vibrational frequencies, Overtones, Combination bands and fermi resonance.

Unit III: Raman and UV-Visible Spectroscopy

Classical and quantum theories of Raman effect, Pure rotational, Vibrational and vibrational-rotational Raman spectra, Selection rules,
Principle of UV-Vis spectroscopy, Beer-Lambert's Law and derivation, Additivity of absorbance, Factors causing deviations from Beer's law, Electronic excitations, involving π, σ and n-electrons, Chromophores and auxochromes, shifts in UV spectroscopy, Instrumentation: Single and double-beam spectrophotometers.

Unit IV: NMR spectroscopy

Principle of Nuclear Magnetic resonance spectroscopy (NMR), Theory, Relaxation process and saturation, Environmental effects on NMR spectra, Chemical shift, Spin-spin splitting, Coupling constant and solvent-effect, Hyphenated technique FT-NMR, Applications to simple molecules (substituted aliphatic and aromatic compounds).

Books Recommended:

1. Quantitative Chemical Analysis; Daniel Harris, Freeman 9th Edn.; 2016
2. Introduction to Spectroscopy, Pavia, Cengage Learning India Pvt Ltd, New Delhi, 5th Edn.; 2015
3. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West, Holt Rinehart and Winston Publications, 4th Edn.; 2014.
4. Analytical Chemistry by G. D. Christian, John Wiley & Sons Inc, Singapore., 7th Edn.; 2013.
5. Principles of Instrumental Analysis, Skoog, Holler, Nieman, 6th Edn.; 2006
6. Spectrometric Identification of Organic Compounds Robert M. Silverstein, John Wiley, 7th Edn; 2005.
7. Introduction to Instrumental analysis: R. D Braun (Tata McGraw-Hill), 1987
8. NMR in Chemistry, MacMillan Ltd, W. Kemp, 1986.
9. Instrumental Methods of Chemical Analysis, G. W. Ewing, McGraw Hill Pub, 5th Edn.; 1985.
10. Fundamentals of Molecular Spectroscopy, C.N. Banwell, E. M.Mccash, Tata McGraw Hill Pub, 4th Edn. 1994.

M.Sc. FIRST YEAR
First Semester
Discipline Centric
Course Title: Mathematics for Chemists
Course Code: PCH-DCE-105

Credits = 3
M.M = 100 (70+30)

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Unit-I: Probability and Vectors

Probability: Variables, Discrete and continuous, Sample space, Event probability, Fundamental counting principles: Permutations and combinations, Binomial probabilities, Probability distribution functions, Probability involving discrete & continuous variables**,** Average values, Distribution moments and variance.
Vectors: Vectors, Dot, Cross and triple products with applications.

Unit-II: Determinants and Matrix Algebra

Determinants, Basic concepts, Types and properties
Matrices: Rectangular, Square, Diagonal & triangular matrices, Trace of a matrix, Addition and multiplication of matrices, Zero & identity matrix, Transpose, Adjoint & inverse of matrices, Special matrices (Symmetric, Skew-symmetric, Hermitian, Skew-Hermitian, Unitary matrices.)
Matrix equations: Homogeneous and non-homogeneous linear equations and conditions for their solutions, Eigen-value problem

Unit-III: Calculus (Differentiation and Integration)

Functions & their continuity and differentiability, Rules for differentiation, Applications of differential calculus including maxima & minima finding (Examples: Maximally populated rotational levels, Bohr's radius, Most probable velocity from Maxwell distribution), Integration, Basic rules for integration, Integration by substitution, Integration by parts, Applications of integral calculus (Kinetics: zero, first, second order reactions)

Unit-IV: Elementary Differential Equations

Partial differentiation, Co-ordinate transformations (Cartesian to spherical polar co-ordinates). Order and degree of differential euations, Homogeneous and non-homogeneous equations. Variable-separable equations: Linear first order differential equations and its solutions. Second order differential equations, Solution by auxiliary equation method. (Applications to chemical kinetics and quantum chemistry).

Books Recommended:

1. Physical Chemistry; Thomas Engel & Philip Reid; Pearson Education 3rd Edn.; 2013
2. Mathematics for Physical Chemistry; R. G. Mortimer; Esevier; 4th Edn.; 2013.
3. The Chemistry Mathematics Book; E. Steiner; Oxford; 2nd Edn.; 2008.
4. Mathematical Method in Physical Science; M. L. Boas, John Wiley and Sons; 3rd Edn.; 2005
5. Mathematical Methods for Scientists and Engineers; D. A. McQuarie; University Science Books; 2003.
7. Basic Mathematics for Chemists; Tebbutt; Wiley; 2nd Edn.; 1998
8. Mathematics for Chemistry; G. Doggett & B. T. Sutcliffe; Longmann; 1995
9. Mathematical Techniques in Chemistry; J. B. Dence; Wiley; 1975.
10. Mathematics for Chemists; C. L. Perrin; Wiley; 1971.

M.Sc. FIRST YEAR
First Semester
Discipline Centric
Course Title: Green Chemistry
Course Code: PCH-DCE-106

Credits = 3
M.M. = 100 (70+30)

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Unit-I: Principles & Concept of Green Chemistry

Concept and Principles, Development of green chemistry- atom economy reactions, Rearrangement reactions, Addition reactions, Atom uneconomic-sublimation elimination-wittig reactions, toxicity measures, Need of green chemistry in our day to day life.

Unit-II: Environmental Performance

Importance of measurement, Lactic acid production, Safer gasoline, Introduction to life cycle assessment, Four stages of life cycle assessment (LCA), Carbon foot printing-green process, Matrics, eco labels- integrated, Pollution, Prevention and control (IPPC)-REACH (Registration, Evaluation, Authorization of Chemicals).

Unit-III: **Green Energy Process**

Design for energy efficiency, Photochemical reactions, Advantages, Challenge faced by photochemical process, Microwave technology on chemistry, Microwave heating, Microwave assisted reactions, Sono chemistry and Green chemistry, Electrochemical synthesis-examples of electrochemical synthesis.

Unit-IV: Renewable Resources

Biomass, Renewable energy, Fossil fuels, Energy from biomass, Solar power, Other forms of renewable energy-Fuel-Cells, Alternative economics, Syngas economy, Hydrogen economy, Bio-refinery chemicals from fatty acids, Polymer from renewable resources, Some other natural chemical resources.

Books Recommended:

1. Green Chemistry in Pharmaceutical Industry, P. J. Dunn. A. Wells, M. T. Williams, Wiley VCH, 2010.
2. Green Chemistry- An Introductory Text; M. Lancester, RSC Publishing, 2nd Edn.; 2010
3. Green Chemistry; Samuel Delvin; IVY Publishing House; Ist Edn.; 2008.
4. Methods and Reagents of Green Chemistry: An Introduction, P. Tundo (Editor), A. Perosa, F. Zecchini, 2007.
5. Green Chemistry- Environment Friendly Alternatives; Rashmi Sangh & M. M Srivastava; Narosa, 2007.
6. Green Chemistry– Environment Benign Reactions, V. K. Ahluwalia, CRC Press, 2007
7. Green Chemistry theory and Practice, P. T. Anastas and J. C. Warner, Oxford University Press, 2000
8. Stream Lined Life-Cycle assessment, T. E. Graedel, Prentice Hall, New Jersey, 1998.

M.Sc. FIRST YEAR
First Semester
Core Course
Course Title: Laboratory Course in Physical Chemistry
Course Code: PCH-CC-107

Credits = 2
M.M. = 100 (70+30)

Potentiometry

i. Determination of strength of an acid by titration with an alkali
ii. Determination of *p*Ka value of a weak acid

Polarimetry

i. Determination of the specific rotation of an optically active compound and determination of unknown concentration from the calibration curve.
ii. Determination of the rate constant of inversion of cane sugar catalysed be HCl.

Calorimetry

i. Determination of heat of neutralization of a strong acid with a strong base.
ii. Determination of heat of neutralization of a weak acid with a strong base.

Spectrophotometry

i. Establishing the validity of Beer-Lambert law.
ii. Determination of composition of a binary mixture through spectrophotometry.
iii. Spectrophotometric titration of Fe (II) vs $KMnO_4$.

Chemical Kinetics

i. Determination of order of reaction between $K_2S_2O_8$ and KI by Initial rates method.
ii. Study of effect of temperature and ionic strength on rate constant of persulphate-iodide reaction.

Viscometery

i. Determination of the coefficient of viscosity of a given liquid and its concentration.
ii. Determination the radius of a molecule.

Books Recommended:

1. Experiments in Physical Chemistry, Schoemaker et al., MGH, 8th Edn.; 2011
2. Experimental Physical Chemistry, Arthur M. Halpern, George C. McBane, Freeman, 3rd Edn.; 2006.
3. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
4. Chemistry Experiments for Instrumental Methods, Sawyer, Heineman, Beebe, Wiley, 1984.
5. Findley's Practical Physical Chemistry, B.P. Levitt, 1973.

M.Sc. FIRST YEAR
First Semester
Core Course
Course Title: Laboratory Course in Inorganic Chemistry
Course Code: PCH-CC-108

Credits = 2
M.M. = 100 (70+30)

Qualitative Analysis

i. Analysis of two cations and anions (macro analysis of elements).
ii. Identification of cations including those of less common elements using semi-micro technique.

Quantitative Analysis

Estimation of a following binary system of cations using gravimetric and volumetric (EDTA or Redox) methods:

i. Copper and Zinc in a given solution
ii. Iron and Nickel in a given solution
iii. Iron and Copper in a given solution

Preparation of Coordination compounds of transition metals:

i. Reinecke salt.
ii. Trinitrotriamine cobalt (III)
iii. Potassium trioxalatomangnate (III)
iv. Ferrous ammonium sulphate.
v. Potassium trioxalatochromate (III)

Separation and Identification of following given mixtures by paper/thin layer chromatography

i. Ni (II) and Co (II).
ii. Co (II) and Ni (II).
iii. Cu (II), Ni (II) and Co (II).
iv. Co (II), Mn (II), Zn (II) and Fe (II)

Books Recommended:

1. Quantitative Chemical Analysis; Daniel Harris, Freeman 9th Edn.; 2016.
2. Inorganic syntheses, Thomas B. Rauchfuss, Vol. 35. Wiley, 2010
3. Advanced Experimental Inorganic Chemistry; Ayodha Singh; Campus Books, 2002.
4. Vogel's Quantitative Analysis Mendham, Denny; Pearson Education, 6th Edn.; 2000
5. Synthesis and Technique in Inorganic chemistry, G. S. Girlomi; R. J. Angleci; University Science Books. 3rd Edn.; 1999.
6. Experimental Inorganic / Physical Chemistry; Mounir A. Malati Horwood/1999.
7. The Synthesis and Characterization of Inorganic compounds W. A Jolly, 3rd Edn.; 1990
8. Advanced Practical Inorganic Chemistry; Adams; Raynor, Wiley; 1965.
9. Thin Layer Chromatography, A laboratory handbook, E. Stahl, Springer Verlag, 2nd Edn.; 1965.
10. Thin-layer chromatography, Justus G. Kirchner, Wiley, 1978.

Syllabus
for
(Open Elective Course)

Open Elective Course

Course Title: Biomolecules

Course Code: PCH-OE-101

Credits = 2
M.M. = 50 (35+15)

Unit-I: Bio-organic Chemistry

Introduction to bioorganic chemistry, Biomolecules, Sugars, Amino acids, Nucleosides, Nucleotides, Nucleic acids, Nitrogenous bases, Polypeptides and proteins, Primary, Secondary, Tertiary and quaternary structure, De- and renaturation of proteins.

Unit-II: Bio-inorganic Chemistry

Introduction, Evidences regarding the presence of inorganic elements in biological systems, Biochemical role of calcium and magnesium, Haemoglobin, Myoglobin, and Vitamin B_{12}, Structure, and biological role, Nitrogen fixation.

Books Recommended:

1. Inorganic Chemistry – Puri, Sharma and Kalia. Milestone publishers, 32nd Edn.; 2014
2. Introduction to Bioorganic Chemistry and Chemical Biology. D. V. Vranket and Gregary Weiss; Taylor and francis. Ist Edn.; 2012.
3. Bio-inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; Ist Edn.; 2009.
4. Organic Chemistry by I. L. Finar Vol-II,. ELBS Publications. 6th Edn.; 2002.
5. Bio-organic Chemistry J. Rohr, Springer, 2000.
6. Bio-organic Chemistry. A Chemical Approach to Enzyme Action, Herrmann Dugas Springer, 3rd Edn.; 1999.
7. Bio-inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; Abbe books, 1977.
8. Inorganic Bio-chemistry, Eichhorn; —Vol. 1 & 2; Elsevier, 1973.

Semester-II

M.Sc. FIRST YEAR
Second Semester
Core Course
Course Title: Metal Clusters and Electronic Spectra of Metal Complexes
Course Code: PCH-CC-201

Credits = 4
M.M.=100(70+30)

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Unit-I: Pi-Acid Complexes

Metal carbonyls, Structure and bonding, Dative overlap, Backbonding (pπ-dπ) synergic interaction, Vibrational spectra of metal carbonyls for bonding and structural elucidation, Important reactions of metal carbonyls, Identification of isomers, IR active bands, Preparation, Bonding, Structure and important reactions of transition metal nitrosyl. Structure of roussins red and roussins black. Nature of M-NO bond, Dinitrogen and dioxygen complexes, Bonding scheme.

Unit-II: Metal Clusters

Occurrence of metal-metal bonds. Structure of some carbonyl metallocenes. (1) Polynuclear compounds (2) Lower halides and oxides. (3) Pre-requisites for the formation of metal-metal bond. (4) Trinuclear compounds (5) Tetranuclear clusters, Metal only clusters. Bonding in metal clusters. Metal carbonyl and metal carbonyl halide clusters, Compounds with metal-metal multiple bonds. Structure and bonding.

Unit-III: Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, Correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), Calculations of Dq, B and β parameters, Charge transfer spectra,
Types of magnetic bodies, orbital and spin effect, Curie equation and Curie Wies law, Determination of magnetic susceptibility, Quenching of orbital concentration, Anomalous magnetic moments, Magnetic exchange coupling and spin crossover.

Unit IV: Symmetry and Group theory

Symmetry elements and operations, Combination of symmetry operations, Groups, Subgroups, Classes, Group multiplication tables, Symmetry point groups, Identification of point groups, Systematic procedure for assignment of point groups to molecules, Symmetry classes and their geometrical significance, Character table (C_{2V}, C_{3V}).

Books Recommended:

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, 2nd Edn.; 2009
2. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 3rd Edn.; 2009
3. Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4th Edn.; 2008.
4. Comprehensive Coordination Chemistry G. Wilkinson, R. D. Gillars and J. A. M. Clevert, 2nd Edn.; 2003.
5. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley 6th Edn.; 1999.
6. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London, Ist Edn.; 1998
7. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon. 2nd Edn.; 1997
8. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier. 2nd Edn.; 1997
9. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons, 1997
10. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series, Ist Edn.; 1991.
11. Chemical Applications of Group Theory, F. A. Cotton, Wiley NY, 3rd Edn.; 1990
12. Magnetochemsitry, R. L. Carlin, Springer Verlag, 1986

M.Sc. FIRST YEAR
Second Semester
Core Course
Course Title: Mechanism of Organic Reactions
Course Code: PCH-CC-202

Credits = 4
M.M. = 100 (70+30)

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Unit-I: Substitution Reactions:

Review and recapitulation of: Aliphatic nucleophillic: S_N1, S_N2, Walden inversion, Mixed S_N1, S_N2, S_NI and SET mechanisms, Effect of leaving group and solvent. Substitution at allylic, benzylic and vinylic carbon atoms.
Aliphatic electrophilic: Mechanisms of reactions involving migration of double bond, Effect of substrate, Leaving group and solvent polarity on reactivity.
Aromatic electrophillic: The Arenium ion mechanism, Energy profile diagrams, Ipso attack, Vilsmeir, Gatterman-Koch, Reimer-Tiemann reactions, Diazonium coupling.
Aromatic nucleophillic: Introduction to different mechanisms of aromatic nucleophilic substitution, S_NAr.

Unit-II: Elimination Reactions

Elimination reactions: The E_1, E_2 and E_1CB mechanisms and orientation of the double bond. Saytzeff and Hoffman's rule. Effect of substrate structure, attacking base, leaving group and medium.
Mechanistic insights of some elimination reactions: Hydro-alkoxy-elimination, *epi*-oxy-elimination, Chugaev elimination, Hoffman elimination, Cope's elimination, Shapiro reaction, Bamford-Stevens reaction, Corey-winter reaction, Ramberg backlund reaction, Boord reaction.

Unit-III: Addition reactions

Addition to carbon-carbon multiple bond: Addition reaction involving electrophiles, (Markownikoff's rule, Peroxide effect), nucleophiles and free radicals, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, Hydroboration, Michael addition.
Addition to carbon-hetero multiple bonds: Overview of reactive carbonyl compounds, Mechanisms of addition of H_2O, HCN, Alcohols, Amines, Addition of Hydrazine, Hydrides to aldehydes and ketones. Mechanism of Wittig, Mannich, Aldol, Cross Aldol, Cannizarro, Knoevenagel, Robinson annulation, Claisen, Dieckman, Benzoin, Perkin and stobbe's reactions.

Unit-IV: Molecular Rearrangement Reactions

Classification and General mechanistic treatment of electrophilic, nucleophilic and free radical moleculer rearrangement. Mechanism of the following rearrangement: Wagner-Meerwin, Pinacol-Pinacolone, Demyanov ring contraction and ring expansion, Benzil-benzillic acid, Favorski, Wolff, Neber, Hoffman, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger.

Books Recommended:

1. Fundamentals of Organic Chemjstry; Solomons; Wiley; 12th Edn.; 2015.
2. Organic Chemistry, John McMurry; Brooks/Cole; 9th Edn.; 2015
3. Advanced Organic Chemistry, Reactions, Mechanism and Structure, Jerry March, 7th Edn.; 2013.
4. Advanced Organic Chemistry; 5th edn.; F. A. Carey and R. J. Sundberg; Springer Plenum; 2007.
5. Organic Chemistry; J. Hornback; Brooks/Cole; 2nd Edn.; 2005.
6. Structure and Mechanism in Organic Chemistry; C. K. Ingold; CBS; 2nd Edn.; 2000.
7. Reaction Mechanism in Organic Chemistry; S. M. Mukherjee and S. P. Singh; Macmillan; 3rd Edn.; 1998.
8. A Guide Book to Mechanism in Organic Chemistry; Peter Sykes; Longman; 6th Edn.; 1996

M.Sc. FIRST YEAR
Second Semester
Core Course
Course Title: Quantum Chemistry & Electrochemistry
Course Code: PCH-CC-203

Credits = 4
M.M. = 100 (70+30)

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Unit-I: Quantum Chemistry-III

Variation theorem, Linear variation principle, Application to Hydrogen atom and Helium atom, Perturbation theory-first order (non-degenerate & degenerate), Application of perturbation method to Helium atom, Chemical bonding, LCAO-MO approximation, H_2^+ molecular ion, Brief introduction to H_2, Molecular term symbols, Valence bond treatment of H_2, Comparison of MO and VB methods in the light of H_2 molecule, Hybridization of orbitals (sp, sp^2 & sp^3).

Unit-II: Quantum Chemistry-IV

Huckel's Pi-MO theory, Application to linear and cyclic polyenes, Pi-electron charge and bond-order. Alternant hydrocarbons, Naphthalene, Heteroatomic conjugated systems. Limitations of Huckel theory, Parisar-Parr-Pople method and extended huckel-method (basic idea), Self-Consistent field method: Hamiltonian and wave function for multi-electron systems, Electronic hamiltonian, Antisymmetrized wave function, Slater-determinant, Hartree-Fock self-consistent field method in the light of system one and two electron integrals.

Unit-I: Electrochemistry-I

Ion-solvent Interactions: Non-Structural (Born) treatment and an introduction to structural (Ion-Dipole, Ion-Quadruple) treatments of ion-solvent interactions, Ion-Ion interactions: Activity and activity coefficients, Debye-Huckel theory of activity coefficients of electrolyte solutions; Derivation of Debye-Huckel limiting law, Validity and extension to high concentrations, Ion-pair formation- Bjerrum model, Debye-Huckel-Onsager conductance equation and brief idea of its extension.

Unit-II: Electrochemistry-II

Metal-electrolyte electrified interfaces, Concept of surface excess, Thermodynamics of electrified interface, Lippmann equation, Electrocapillary curves, Methods for determination of surface excess. Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, Recent advances. Semiconductor electrodes: Structure of semiconductor/electrolyte interface, Theories of heterogeneous electron transfer: Electron transfer at electrified interface at and away from equilibrium, Butler-Volmer Equation, Low and high field approximations, Significance of transference-coefficient.

Books Recommended:

1. Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7th Edn.; 2013.
2. Molecular Electronic-structure Theory, Helgaker et al., 2013
3. Quantum Chemistry, Prasad, New Age Publishers, 4th Edn.; 2010 (Reprint 2014).
4. Molecular Quantum Mechanics- P. W. Atkins and R. S. Friedmann, Oxford, 5th Edn.; 2010.
5. Introduction to Quantum chemistry; A. K. Chandra; Tata McGraw Hill; 1998.
6. Physical Methods for Chemists, R. S. Drago, Saunders College Publishing; 2nd Edn.; 1992.
7. Electrochemistry, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH. 2nd Edn.; 2007
8. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, Ist Edn.; 2007.
9. An introduction to Electrochemistry, S. Glasstone, Maurice Press, 2007
10. Physical Chemistry- P. W. Atkins, ELBS, Oxford, 8th Edn.; 2006.
11. Modern Electrochemistry 1, 2A, J. O. Bokris and A. K. Ready, Kluwer Academic/plenum Publishers, New York. 2nd Edn.; 2002,
12. Electrochemical methods, Fundamentals and Methods, A. J. Bard, L. R. Faulkner, Wiley, 2nd Edn.; 2002
13. Physical Electrochemistry-Fundamentals, Techniques and Applications, E. Gileadi, Wiley-VCH, 2011.
14. Physical Chemistry- A Molecular Approach- D. A. Mc Quarie & J. D. Simon, 1997.

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M.Sc. FIRST YEAR
Second Semester
Discipline Centric
Course Title: Chromatographic Techniques
Course Code: PCH-DCE-204

Credits = 3
M.M. = 100 (70+30)

Unit-I: Thin-Layer Chromatography

Introduction and principle, Types and selection of stationary phases (adsorbents) and mobile Phases, Methods of plate development; Detection of spots; Performance characteristics of Thin-Layer plates, Retardation and retention factor, Plate heights, High-performance thin-layer chromatography, Application
Chiral chromatography: Chiral derivatization, Chiral mobile-phase, Chiral stationary phases, Mechanism of chiral interactions, Applications.

Unit-II: Size Exclusion and Ion Exchange Chromatography

Introduction and principle, Gels, Theoretical basis, Exclusion limit, Total permeation and selective permeation regions. Relation between elution volume and molecular weight, Fractionation in a complex mixture, Packing materials and applications,
Introduction to ion-exchange chromatography, Types of ion exchange materials, Mechanism of ion exchange, Ion exchange equilibrium, Volume and ion exchange capacity, Ion chromatography. Distinction between ion-exchange and ion chromatography, Applications IEC for separation of biological molecules.

Unit-III: High Performance Liquid Chromatography (HPLC)

Introduction; Principle, Theory and instrumentation, Plate theory, Rate theory, Van-Deemter-Equation, Resolution, Retention time and other basic parameters, Basic difference between HPLC and conventional liquid-chromatography, Packing materials and equipments, Detectors, Advantages and Applications, Reverse phase HPLC and normal phase HPLC, Brief Introduction to hyphenated LC-MS technique.

Unit-IV: Gas Chromatography

Introduction and principle, Instrumentation: Columns and stationary phases, Detectors:- TCD, FID and Electron Capture Detector, Factors Affecting the efficiency of the column, Van-Deemter Equation, Qualitative and qantitative analysis based on peak height and peak area, Brief introduction to hyphenated GC-MS technique.

Books Recommended:

1. Analytical Chemistry by G. D. Christian, John Wiley & Sons Inc, Singapore., 7th Edn.; 2013.
2. Gas Chromatography and Mass Spectrometry: A Practical Guide, O David Sparkman, Zelda Penton and Fulton G. Kitson, Elsevier, 2nd Edn.; 2011.
3. Introduction to Modern Liquid Chromatography: L. R. Snyder& J. J. Kirkland (John Wiley & Sons, New York). 3rd Edn.; 2009
4. Chromatography: Concepts and Contrasts, James M. Miller, Wiley, 2nd Edn.; 2009.
5. Principles of Instrumental Analysis, Skoog, Holler, Nieman, 6th Edn.; 2006
6. Principles and Practice of Analytical Chemistry by F. W. Fifield and D. Kealey, Blackwell Science Ltd, New Delhi 5th Edn.; 2004.
7. Handbook of Instrumental Techniques for Analytical Chemistry, Editor, F. Settle, Pearson Education Inc, New Delhi. Low Price Edn, 2004.
8. Instrumental Methods of Analysis, Willard, Merit, Dean and Settle, CBS Publishers and Distributors, 7th Edn.; 2004.
9. Chiral Separations by liquid chromatography and related technologies, Hassan Y. Aboul-Enein, Imran Ali, CRC press, 2003.
10. Chromatography and Separation Science By Satinder Ahuja McGraw Hill Pub, 5th Edn.; 1985.
11. Chromatographic Methods by A.Braithwaite and F.J.Smith by Kluwer Academic Publishers 5th Edn,;1999

M.Sc. FIRST YEAR
Second Semester
Discipline Centric
Course Title: Bioinorganic Chemistry
Course Code: PCH-DCE-205

Credits = 3
M.M. = 100 (70+30)

Unit-I: Metal ions in Biochemical Systems

Introduction to bio-inorganic chemistry, Concept of essentiality, Criteria and classification of essential elements as per their role in living systems, Bulk metals and trace metals, Role of alkali and alkaline earth metals in biosystems, Metal ion toxicity, Na^+-K^+ pump, Biochemistry of iron (transport and storage), Application of radioactive elements for biosystems.

Unit-II: Metalloporphyrins and Respiration

Metalloporphyrins, Cytochromes (Cytochromes C, Cytochrome C-oxidase, Cytochrome P-450). Dioxygen transport (haemocyanin and hemoerythrin), Structure and physiological role of hemoglobin and myoglobin, Bohr Effect and cooperativity, Chloride effect.

Unit-III: Electron Transport in Biosystems

Electron transport in biosystems, Iron-Sulfur proteins, Ferredoxins, Rubredoxin, Blue copper proteins, Photosynthesis (PS I and PS II), Z-scheme, Structure of chlorophyll a and b, Manganese complex, Becterio- chlorophyll.

Unit-IV: Enzymes and medicinal Chemistry

Enzymes and co-enzymes, Structure and function of carboxypeptidase A, Carbonic anhydrase, Xanthine oxidase, Phosphatase, Vitamin B-12, Nitrogen fixation, Biochemical basis of essential metal deficient diseases and their therapies (Iron, Zinc, Copper and Manganese). Chelate therapy, Anticancer drugs-cisplatin.

Books Recommended:

1. Inorganic Chemistry – Puri, Sharma and Kalia. Milestone publishers, 32nd Edn.; 2014
2. Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4th Edn.; 2008.
3. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
4. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.
5. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
6. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden; 1991
8. A Text book of Medicinal aspects of Bioinorganic Chemistry; Das; CBS; 1990.
9. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
10. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976
11. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
12. The Inorganic Chemistry of Biological processes; Hughes ; Wiley; 2nd Edn.; 1973.

M.Sc. FIRST YEAR
Second Semester
Discipline Centric
Course Title: Conducting Polymers
Course Code: PCH-DCE-206

Credits = 3
M.M. = 100 (70+30)

Unit-I: Basic Concepts

Basics of conducting polymers, Historical background. Classification of electrochemically active polymers, Redox polymers, Electronically conducting polymers (Intrinsically Conducting Polymers—ICPs), Electronically conducting polymers with built-in or pendant redox functionalities, Copolymers, Composite materials, Applications of conducting polymers.

Unit-II: Synthesis

Electrolytic conduction, Electrodes and mechanism; Electrochemical-synthesis of derivatives of poly-pyrrole, Polythiophene, Polyazulene, Polycarbazole, inser inorganic examples.

Unit-III: Semiconducting and Metallic Polymers

Introduction and structural basis for semiconducting, metallic polymers and organic meta-polymers- synthetic routes, isomers and electronic structure of polyacetylene, Poly-*p*-phenylene, Polypyrrole, Polythiophene, inser metallic examples

Unit-IV: Doping and Catalysis

Introduction, Electrochemical doping, Role of reduction and oxidation potential in doping, Polyacetylene as electrode materials.
Introduction to catalysis, Catalytic properties of conducting polymers, Catalysis of electron donor-acceptor complexes. Electrocatalysis by semiconducting polymers.

Books Recommended:

1. Conducting Polymers; A New Era in Electrochemistry, Gyorgy Inzelt, Springer-Verlag Berlin Heidelberg 2nd Edn.; 2012.
2. Conductive Electroactive Polymers, Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, CRC Press, 3rd Edn..; 2008
3. Conductive Polymers and Plastics, Larry Rupprecht, Elsevier, Ist Edn.; 2000.
4. Handbook of Conducting Polymers, Terje A. Skotheim, Ronald L. Elsenbaumer, John R. Reynolds, Marcel Dekkar, 2nd Edn.; 1997.
5. Handbook of Organic Conductive Molecules and Polymers, Four Volume Set, Hari Singh Nalwa (Editor), Wiley, 1997.
6. Organic Conductors, Jean-Pierre Farges, Marcel Dekkar, 1994
7. New Concepts in Polymer Science, Polymeric Composites, Raymond B Seymour, VSP, 1990.
8. Electrically Conductive Organic Polymers for Advanced Applications David B Cotts, Z Reyes, 1987.

M.Sc. FIRST YEAR
Second Semester
Core course
Course Title: Laboratory course in Organic Chemistry
Course Code: PCH-CC-207

Credits = 2
M.M. = 100 (70+30)

Unit-I: Organic Preparations

1. Preparation of dibenzal acetone from benzaldehyde.
2. Preparation of adipic acid by chromic acid oxidation of cyclohexanol.
3. Preparation of caprolactum.
4. Preparation of phenol formaldehyde resin.
5. Preparation of cinnamic acid by perkin reaction.

Unit-II: Qualitative Analysis.

1. Detection of elements: nitrogen, sulphur and halogens.
2. Detection of functional groups: detection of carbohydrates, Unsaturation, Carboxylic acids, Carbonyl compounds, Phenols, Alcohols, Halides, Amines, Amides, Imides, Ureas, Thioureas, Nitrocompounds and hydrocarbons.
3. Separation and identification of binary organic compounds using physico-chemical methods.

Books Recommended:

1. Organic Chemistry Lab Manual N. S. Gnanapragasam and B. Ramamoorthy, S. Visvanathan Printers & Publishers, 2010.
2. Comprehensive Practical Organic Chemistry; V. K. Ahluwalia and Renu Aggarwal; University Press; 2000
3. Advanced Practical Organic Chemistry; N. K. Vishnoi; Vikas; 2nd Edn.; 1999.
4. Vogel's Textbook of Practical Organic Chemistry; A. R. Tatchell; ELBS; 5th Edn.; 1996.
5. Experiments and Techniques in Organic Chemistry; D. Pasto, C. Johnson and M. Miller; Prentice-hall; 1992.
6. Microscale and Macroscale Organic Experiments; K. L. Williamson; D. C. Heath and Co. 1989.

M.Sc. FIRST YEAR
Second Semester
Core Course
Course Title: Laboratory course in Analytical Chemistry
Course Code: PCH-CC-208

Credits = 2
M.M. = 100 (70+30)

Unit-I: pH-metry

i. Determination of strength and pKa value of a weak acid by titration with an alkali.
ii. Titration of a dibasic acid with alkali to find its pKa values.

Unit-II: Ion Exchange

i. Determination of Ion-exchange capacity of resin (cationic and anionic).
ii. Separation of Zn and Cd by ion-exchangers.

Unit-III: Chromatography

i. Column chromatographic separation of cis and trans azobenzene, determined spectrophotometrically.
ii. Separation of amino acids by thin layer and paper chromatography.

Unit-IV: Spectroscopy

i. Extraction of caffeine from tea leaves, characterization by IR.
ii. Determination of iron in pharmaceutical samples by visible spectrophotometry**.**

Unit-V: Quantitative analysis

i. Determination of iodine value and saponification value of edible oils.
ii. Determination of copper and zinc in brass.
iii. Determination of metal ions by flame photometry (sodium, potassium, sodium and potassium in a mixture).

Books Recommended:

1. Environmental Chemistry, A. K. De, 7th Edn.; 2010.
2. Practical Pharmaceutical Chemistry, part-2, Beckette, Stenlake, 4th Edn.; 2001.
3. Analytical Chemistry Thoery and Practice, R. M. Verma .CBS Publishers & Distrbutors, 3rd Edn.; 2000.
4. Vogel's Quantitative Analysis Mendham, Denny; Pearson Education 6th Edn.; 2000
5. A textbook of Practical Organic Chemistry, A. I. Vogel, 5th Edn.; 1996.
6. Standard methods of Chemical Analysis, F. J. Welcher, 6th Edn.; 1962.
7. Experiments in Chemistry, D. V. Jagirdar, Himalaya publication.

Syllabus
for
(Open Elective Course)

Open Elective Course

Course Title: Introduction to Nanotechnology

Course Code: PCH-OE-201

Credits =2

M.M. = 50 (35+15)

Unit-I: Nanotechnology

Introduction to nano science and nanotechnology**,** Defining nanoscale science, Properties of materials at nanoscale: Optical, electrical, thermal, mechanical and magnetic.
Carbon Nanotubes (Properties and Applications).

Unit-II: Methods of Preparation

Top down approach and bottom up approach for synthesis of nanomaterial, Ball milling, Sol-gel method, Solution based method, Solvo-thermal synthesis, and Photochemical synthesis.

Books Recommended:

1. Nanotechnology, J. Ramsden, Elsevier, Ist Edn.; 2011.
2. Nanotechnology Importance and Application, Fulekar, I K International Publishing House, 2010.
3. Springer Handbook of Nanotechnology, B. Bhushan (Editor), 3rd Edn.; 2010.
4. Essentials of Nanotechnology. J Ramsden, 2009.
5. Nanotechnology Fundamentals and Applications, Manasi Karkare, I K International Publishing House, 2008.
6. Introduction to Nanoscale Science and Technology, M. Ventra, S, Evoy, J.R. Heflin. Springer; 2004.

Semester-III

M.Sc. SECOND YEAR
Third Semester
Course Title: Organometallic Chemistry
Course code: PCH-CC-301

Credits = 4
M.M. = 100 (70+30)

Unit—I: Sigma bonded Organometallic Compounds

Classification, Stability, Routes of synthesis, Reactions, Structure and bonding. Decomposition pathways: α and β hydrogen transfer. Intramolecular elimination of alkane. Stability from bulky substituents, Agostic alkyls.

Unit—II: π-bonded Organometallic Compounds

Classification, Synthesis, Structure and bonding in Metal—alkynes, allyIs, 1,3-butadiene and cyclobutadiene complexes Sandwich compounds: General characteristics; Classification, Synthesis, Reactions, Structure and bonding of cyclopentadienyl complexes with special reference to ferrocene.

Compounds with transition metal—carbon multiple bonds, Alkylidene and alkylidyne synthesis, Structural characteristics, Nature of bonding.

Unit—III: Catalytic Processes involving Transition Metal Organometallic Compounds: -

Mechanistic aspects: Oxidative addition, Insertion reactions and reductive elimination. Hydrogenation, Hydroformylation, Oxidation, Isomerization and Zeigler-Natta-- polymerization of alkenes.

C-C coupling reactions- Suzuki and Heck, Grubbs catalyst. Activation of small molecules like CO, CO_2 and alkanes.

Unit—IV: Fluxional Organometallic Compounds:-

General characteristics, Rates of rearrangement and techniques of study. Classification of fluxional organometallic compounds. Some simple examples of non-rigid molecules in 4 and 5 coordination geometries. Fluxionality and dynamic equilibria in compounds such as 2 -olefin, 3 -allyl and dienyl complexes.

Books Suggested

1. Principles and applications of organotransition metal chemistry, Collman J. P., Hegsdus L. S., Nortan J. R. and Finke R. G., University Science Books.
2. The Organometallic chemistry of the transition metals, R. H. Crabtree, John Wiley.
3. Metallo-organic chemistry, Pearson A.J., Wiley.
4. Organometallic chemistry, Mehrotra R. C. and Singh A., New Age International.
5. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
6. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
7. Inorganic Chemistry; 4* edn; Huheey; Harper & Row; 1990.
8. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
9. Chemistry of elements, NN Green Wood, Elsevier.

M.Sc. SECOND YEAR
Third Semester
Core Course
Course Title: Pericyclic Reactions and Organo-Photochemistry
Course Code: PCH-CC-302

Credits = 3
M.M = 100 (70+30)

Unit-I: Pericyclic reactions-I

General introduction, Definition and classification of pericyclic reactions. Molecular orbital symmetry, Frontier molecular orbital concept (FMO), HOMO, LUMO and SOMO: Frontier molecular orbitals of various π-electron systems including ethene, 1, 3-butadiene, 1,3,5-hexatriene and allylic systems. Woodward Hoffman rules for pericyclic reactions.

Unit-II: Pericyclic reactions-II

Cycloadditions: Thermal and photochemical 2+2 and 4+2 cycloadditions, Suprafacial and antrafacial cycloadditions.
Electrocyclic Reactions: Thermal and photochemical electrocyclic reactions of 4n and 4n+2 systems and their stereochemical aspects, Conrotatory and disrotatory motions.
Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts, Cope and claisen rearrangements, Suprafacial and antrafacial shifts of hydrogen, Biological pericyclic reactions.

Unit-III: Photochemistry-I

Types of photochemical excitations, Direct and indirect excitations, The fate of excited molecule, Singlet and triplet states and their lifetimes, Jablonski diagram, Transfer of excitation energy: sensitization and quenching, quantum yield, Different types of photochemical reactions,
Photochemical reactions of alkenes: Geometrical isomerization reactions, Dimerization and cyclization reactions, Photochemical reactions of 1,3-butadiene, rearrangements of 1,4 and 1,5-dienes.

Unit-IV: Photochemistry-II

Photochemical reactions of saturated cyclic and acyclic carbonyl compounds, Norrish type-I and Norrish type-II reactions, Paterno-Buchi reaction.
Photochemical reactions of α, β-unsaturated carbonyl compounds (H-abstraction and isomerization to β,γ-unsaturated carbonyl compounds).
Light induced isomerizations of benzene and its alkyl derivatives, Nucleophilic photosubstitution reactions of aromatic compounds, Photo-Fries rearrangement of aryl esters and anilides.
Photochemistry of vision, Photolysis of organic nitrites.

Books Recommended:

1. Introductory Photochemistry, A. Cox and T. Kemp (McGraw Hall-1971).
2. Organic Photochemistry, 2nd Ed., J. Coxon, and B. Halton (2ndEd.CambridgeUniversity press-1987).
3. Fundamentals of photochemistry, Rohtagi & Mukherjee (Wiley Eastern-1992).
4. Advanced Organic Chemistry, Reactions, Mechanism and Structure, 4th Ed., Jerry March (Wiley, 1999).
5. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole, 2000).

M.Sc. SECOND YEAR
Third Semester
Course Title: Thermodynamics and Solid state Chemistry
Course code: PCH-CC-303

Credits = 4
M.M. = 100 (70+30)

Unit I: Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics. Entropy and entropy change, Helmoltz and Gibbs free energy, change in free energy, Gibbs-helmholtz equation. Partial molar properties, Partial molar free energy & chemical potential, partial molar volume and partial molar heat content and their significances, Determination of these quantities, Concept of fugacity and determination of fugacity. Application of phase rule to two component systems, eutectics.

Unit II: Interface Thermodynamics

Liquid Surface: Surface tension, pressure difference across curved surfaces (Laplace equation), vapor pressure of droplets (Kelvin equation), Capillary condensation, Solid liquid interface: Contact angle, young's equation. Wetting, wetting as contact angle phenomena, Thermodynamics of Interfaces: surface excess, surface tension and thermodynamic parameters, Gibbs adsorption isotherm. Solid surfaces: Adsorption at solid surfaces, adsorption models, Langmuir adsorption isotherm, BET adsorption isotherm and its use in estimation of surface area, Adsorption on porous solids.

Unit III: Solid State Chemistry-I

Point groups, Space groups. Lattice Planes and Miller indices; Bragg equation, Debye-Scherrer method of X-ray structural analysis. Identification of cubic unit cells from systematic absences in diffraction pattern. *S*tructure factor and its relation to intensity and electron density. Crystal structure of Perovskite ($SrTiO_3$), and Rutile (TiO_2).

Crystal defects and their types, Point defects: Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defect formation, Colour centres, Dislocations and their types

Unit IV: Solid State Chemistry-II

Band theory of solids

***Semiconductors*:** Intrinsic & extrinsic semiconductor (n-type & p-type), temperature dependence of charge carriers, p-n junction- devices based on p-n junction (tunnel diode, injection laser).

Super conductors: Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, absorption of electromagnetic radiations and Josephson effect. BCS theory of superconductivity. Applications.

Luminescence and Lasers.

Liquid crystals and their applications

Books Recommended:

1. Physics and Chemistry of Interfaces, H-J, Butt, K. Graf and M. Kappl, 2nd Edition, Wiley- VCH VerlagGmbh and Co. KGaA, 2006.
2. Physical Chemistry - P. W. Atkins, ELBS Oxford, 1997.
3. Physical Chemistry - A Molecular Approach - D. A. McQuarie& J. D. Simon, University Science Books, 1997.
4. Introduction to Solids, Azaroff, Tata McGraw,1993.
5. Solid State Chemistry and its Applications, A R West, Wiley,1989.
6. Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders college, 2001.
7. Elements of Solid state Physics, J.P. Srivastava, Prentice Hall of India, 2003.

M.Sc. SECOND YEAR
Third Semester
Course Title: Polymers and Nanotechnology
Course code: PCH-CC-304

Credits = 3
M.M. = 100 (70+30)

Unit-I: Chemistry of Polymerization

Importance of polymers; Basic concepts: Monomers, Repeat units, Degree of polymerization, Classification of polymers: skeletal structures, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, Properties and polymerization mechanism Chain polymerization, Step polymerization, Copolymerization, Miscellaneous polymerization reactions, Polymerization techniques-Bulk, Solution, Suspension, Emulsion polymerization, Melt poly-condensation, Solution poly-condensation, Application of polymers.

Unit-II: Polymer Characterization and Properties

Polydispersion and average molecular weight concept: Number, Weight & viscosity average molecular weights, Measurement of molecular weights: End-group, Membrane osmometry light scattering and viscometry, Polymer crystallization, Morphology and chain tacticity; Melting (Tm) and glass transition(Tg) temperature, Efects of molecular weight, dilutents, Chemical structure, Branching and cross linking, Relationship between Tm and Tg; Thermal analysis and visco-elastic properties.

Unit-III: Nanotechnology I

Nanoscience and nanotechnology, Nanostructures in nature, Surface effects of nanomaterials, Surface plasmon resonance, Quantum size effects, Effect of size on properties, reactivity, optical, electrical, and magnetic properties.
Application of nanomaterials in medicine, Nanomaterials for energy sector, Nanomaterials in food, Nanomaterials for the environment, Nanomaterials in automobiles.

Unit-IV: Nanotechnology II
Nanomaterials synthesis, Top-down and bottom-up approaches,
Solvothermal synthesis, Hydrothermal synthesis, Reverse micellar/Micro-emulsion method, Reverse micelles as nano reactors, Mechanism for nanoparticle synthesis inside the reverse micelles, Co-precipitation, Sol-Gel Method, Brief introduction and characterization techniques for Nanomaterials

Books Suggested:

1. Textbook of Polymer Science, F.W. Billmeyer Jr., John Wiley & Sons, Inc., 2000.
2. An Introduction to Polymer Chemistry, W.R. Moore, University of London Press Ltd., London.
3. Introduction to Polymers, R.J. Young and P.A. Lovel, Chapman & Hall, London.
4. Polymer Chemistry-An Introduction, R.B.Seymour & C.E. Carraher, Jr., Marcel Dekker, Inc., New York.
5. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedahr, New Age International(P) Ltd. Publishers, 2001.
6. Sperling LH, *Introduction to Physical Polymer Science*, Fourth Edition, Wiley-Inter science (2005)
7. Chanda M, *Introduction to Polymer Science and Chemistry, A Problem Solving Approach*, CRS Press (2006)
8. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
9. Nano Materials, B. Viswanathan, Narosa Publications, 2009.
10. Nano: The Essentials, T. Pradeep, Tata Mcgraw Hill, 2009.
11. Chemistry of Nanomaterials: Synthesis, Properties and Applications by C.N.R. Rao, A.Muller and A. K. Cheetham (eds.), Wiley-VCH, Weinheim, 2004.
12. Nanoscale Materials by Luis M. Liz-Marzan and Prashant V.Kamat, Kluwer Academi Publishers (Boston), 2003.
13. Physical Principles of Electron Microscopy: An introduction to TEM, SEM and AFM by R.F. Eqerton, Springer, 2008.

M.Sc. SECOND YEAR
Third Semester
Course Title: Spectroscopy of Organic Compounds
Course code: PCH-DCE-305

Credits = 3
M.M. = 100 (70+30)

Unit-I: Ultraviolet and Infrared Spectroscopy

Ultraviolet absorption spectra of dienes (homo and heteroannular), Enones, Carbonyl compounds, Unsaturated carbonyl compounds, Aromatic and heteroaromatic compounds, Effect of solvent on electronic transitions, Effect of conjugation on ultraviolet spectra, Woodward-Fieser rules, Application and limitation, Kuhn's rule, Application to conjugated polyenes.

Introduction, Instrumentation and sample handling, Characteristic vibrational frequencies of alkanes, Alkenes, Alkynes, Alcohols, ethers, Phenols, Amines, Aldehydes, Ketones, Acids, Anhydrides, Esters, Lactones, Amides and conjugated carbonyl compounds, Effect of hydrogen bonding and solvent on vibrational frequencies in IR spectra, Overtones, Combination bands and fermi resonance, FT-IR.

Unit-Il: Mass Spectrometry

Introduction, Instrumentation, A typical mass spectra, molecular ion peak, Ion production, EI, CI, FD, FAB, ESI and MS/MS methods, Role of isotopes in mass spectrometry, Fragmentation pattern of various classes of organic compounds, Metastable peak, Nitrogen rule, High resolution mass spectrometery. Fragmentation pattern, Initial ionization event, α-cleavage, Inductive cleavage, Two bond cleavage, Retro-Diels Alder cleavage and McLafferty rearrangement.

Unit-III: Nuclear magnetic resonance spectroscopy

Proton NMR Spectroscopy
Shielding effect, Chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, Phenols, Enols, Carboxylic acids, Amines, Amides and mercapto). Chemical exchange, Effect of deuteration, Complex spin-spin interactions between two three, four and five nuclei (first order spectra) virtual coupling, Stereochemistry, Hindered rotation karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, Nuclear magnetic double resonance, Contact shift reagents, Solvent effect, Fourier transform technique, Nuclear overhauser effect (NOE). Bio-chemical applications of NMR (examples).

Unit-IV: Carbon-13 NMR Spectroscopy

General considerations, Chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromtic and carbonyl carbon), Coupling constant, Two dimensional NMR spectroscopy- COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

Books recommended:
1. Spectrometric identification of Organic Compounds.5th Ed., R. M. Silverstein, G. C. Bassler and T. C. Morill. (Jhon Wiley-1991).
2. Introduction to NMR Spectroscopy, R. J. Abraham. J. Fisher and P. Loftus (Wiley- 1991)
3. Applications of absorption spectroscopy of Organic Compounds, J. R. Dyer (Prentice Hall-1991).
4. Spectroscopic Methods in organic Chemistry, D. H. Williams; I. Fleming (Tata- McGraw Hill-1988).
5. Introduction to Spectroscopy. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan. Cengage Learning, 2008

M.Sc. SECOND YEAR
Third Semester
Course Title: Inorganic Spectroscopy
Course Code: PCH-DCE-306

Credits = 3
M.M. = 100 (70+30)

Unit-I: NMR Spectroscopy

Multinuclear NMR spectroscopy in inorganic chemistry. Paramagnetic shift in ^{1}H NMR spectra, ^{31}P NMR, ^{11}B NMR ^{19}F NMR (Splitting pattern and spectrum). Exchange process in solution Spin-spin coupling, Magnetic resonance imaging (MRI), MRI contrast agents, Brief introduction of solid-state NMR.

Unit-II: Mossbauer Spectroscopy (MB Spectroscopy)

Technique of Mossbauer Spectroscopy, Gamma-ray fluorescence, Gamma radiation source, Doppler effect, Isomer shift, quadrupole splitting, Magnetic hyperfine splitting, Applications in inorganic complexes (Bonding and Structure of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+}, Recognition of nature of M-L bond, Coordination compound, Structure and oxidation state.

Unit-III: Electron Spin Resonance (ESR/EPR Spectroscopy)

Principle of ESR spectroscopy. Hyperfine structure in ESR spectra, Hydrogen atom, Methyl radical, $(SO_3)_2NO^-$ anion, Fermi-contact interaction, *g*-factor: g_{11} *and* $g_{\perp}$. Applications of ESR, Spin labels, McConnell equation, Isotropic and anisotropic systems, Hyperfine splitting, Spin hamiltonian, Kramer's degeneracy and Zero field splitting. ESR Spectra of some transition metal complexes and biomolecules.

Unit-IV: Nuclear Quadrupole spectroscopy (NQR)

NQR Isotopes, Basic theory of quadrupole spectroscopy, Quadrupole nuclei, Nuclear quadrupole moment, Electric field gradient (EFG), Nuclear Quadrupole Coupling constant, Effect of applied magnetic field (Zeeman effect), Towns-Dailey Theory, Applications of NQR and NQR spectra of $^{14}N_7$, $^{11}B_5$.

Books Recommended

1. NMR, NQR and EPR and Mossbauer Spectroscopy in Inorganic Chemistry; Parish and Elis, H; 1990.
2. Nuclear Quadrupole Resonance Spectroscopy, Das, T. P. and Hahn, E. L. Academic Press; 1958.
3. Principles of Physical Chemistry; Pure, B. R. Sharma, L. R. and Pathiana, M. S; 47th Edition.
4. Spectroscopy in Inorganic Chemistry; Vol I and II; Rao, Ferraro; Academic Press; 1970.
5. Structural Methods in Inorganic Chemistry; 2nd edn; Ebsworth, E. A. V and Rankin, D. W. H; ELBS; 1991.
6. Inorganic Chemistry; Catherine, E. H and Sharpe, A. G; 2nd Edition, Pearson.

M.Sc. SECOND YEAR
Third Semester
Course Title: Chemo-informatics
Course code: PCH-DCE-307

Credits = 3
M.M. = 100 (70+30)

Unit-I: Representation of Molecules and Chemical Reactions

Nomenclature; Different types of Notations; SMILES coding; Matrix Representations; Structure of Molfiles and Sdfiles; Libraries and toolkits; Different electronic effects; Reaction classification

Unit-II: Searching Chemical Structure

Full structure search; sub structure search; basic ideas; similarity search; Three dimensional search methods; Basics of Computation of Physical and Chemical Data and structure descriptors; Data visualization.

Unit-III: Computer Assisted Virtual screening design

Structure Based Virtual Screening- Protein Ligand Docking, Scoring Functions for Protein Ligand docking, Practical aspects of structure based Virtual Screening; Prediction of ADMET Properties, 2 D and 3D data searching, Chemical databases, Role of computers in Chemical Research.

Unit-IV: Application of Chem-informatics in Drug Design

Quantitative Structure-Property Relations;
Descriptor Analysis; Computer Assisted Structure elucidations; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Design of Combinatorial Libraries; Ligand- Based and Structure Based Drug design

Books Recommended:

1 Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Chem-informatics, Academic Publisher, Netherlands, 2003
2. Lisa B. English (Editor), Combinatorial Library Methods and Protocols, Humana Press Inc, Volume:201, 2002
3. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition, 2006

M.Sc. SECOND YEAR
Third Semester
Course Title: Advanced Laboratory Course
Course Code: PCH-CC-308

Credits = 4
M.M. = 100 (70+30)

Spectrophotometry

1. To study the complexation reaction between Fe (III) & salicylic acid.
2. Determine the dissociation constant of an indicator by spectrophotometric method.
3. Determination of Iron (II) with 1,10-Phenanthroline.
4. Determination of Phosphate by Molybdenum blue method.
5. Estimation of aspirin from given tablet by Spectrophotometry
6. Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard material

Potentiometry

1. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
2. Determination of formation constant of Ag-NH_3 complex
3. Standardization of an Iron (II) solution with a standard dichromate solution over Pt & Calomel assembly.
4. Estimation of iodide with Standard AgNO3 over Pt & Calomel assembly using I - \ I2 redox couple.
5. Simultaneous determinations of chloride and iodide ions with Standard AgNO3 over Ag-Glass electrode assembly

Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.
3. To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
4. To determine the basicity of sodium potassium tartarate by conductometric method.

Kinetics

Study the kinetics of reaction between potassium persulphate and potassium iodide:
a) Determine the rate constant and order of reaction.
b) Study the influence of ionic strength on the rate constant.

Viscometry

Determination of Mol. Mass of a Polymer (Polyvinyl alchol) using viscosity method.

Polarimetery

1. Determination of specific, molecular and intrinsic rotation of an optically active compound
2. Study of inversion of cane sugar in presence of acid.

pH-metric Titrations

Purity of Acetyl Salicylic acid (Aspirin) in a commercial tablet by pH Titration.

Chromatography

1. Separation of organic compounds by column chromatography
2. Analysis of Paracetamol by HPLC
3. Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
4. Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6]\ Cl_3$ and $[Co\ (NH_3)_5\ Cl]\ Cl_2$ on Silica column.

Synthetic Preparations

1. Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
2. Preparation of trans dicholoro bis (ethylenediamine), cobalt (III) chloride and its conversion to cis-isomer.
3. Synthesis of aspirin and its characterization by physical and spectroscopic methods.
4. Synthesis of paracetamol and its characterization by physical and spectroscopic methods.
5. Beckmann rearrangement.

Extraction/Estimation of Organic compounds from natural sources

1. Isolation of lycopene and beta-carotene from tomato, Characterization of lycopene/P-carotene by UV -absorption process.
2. Isolation of limonene from its natural source and physicochemical analysis.
3. Assay of lemon for citric acid and vitamin-C
4. Assay of coke (soft drink)
5. Estimation of Nitrogen from Fertilizer sample
6. Estimation of Uric acid in the given sample of blood serum
7. Estimation of phosphoric acid in soft drink by molybdenum blue method.
8. Estimation of BOD and DO in Waste Water Sample
9. Estimation of acid value of oil

Books Recommended

1. Practical Physical Chemistry ----Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. ---- Schoemaker et al. (MGH, 2003)
4. Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
5. Synthesis and characterization of Inorganic compounds W.AJolly
6.Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
7. Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
8. Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
9. Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.
10. Practical Clinical biochemistry methods and interpretations, R.Chawla, J.P. Bothers Medical Publishers (P) ltd., 1995.
11. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
12. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn
13. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson Education Pvt. Ltd., New Delhi
14. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
15. Quantitative Chemical Analysis; Kolthoff, sandell Meehan and Bruckestein; Mcmillan Co., London, 1969

Syllabus
for
(Open Elective Course)

Open Elective Course

Course Title: Drugs and Chemotherapy

Course Code: PCH-OE-301

Credits = 2
M.M. = 50 (35+15)

Unit-I: Drugs

Introduction, Classification of drugs, Effect of drugs, Drug resistance, Action of chemotherapeutic and pharmacodynamic agents, New development in drug research-peptide drugs, Gene therapy and antisense drugs. Introduction to drug design.

Unit-II: Chemotherapy

Introduction, Analgesics, Antipyretics, Antiflammatory drugs (mode of action and uses), Sulpha drugs; General mode of action of sulpha drugs and their uses, Antibiotics, Chloroamphenicols their mode of action and uses, Drugs for cardiovascular diseases, Antimalarial drugs, Artemisinin.

Books Recommended:

1. Organic Chemistry, Bhupinder Mehta and Manju Mehta, 2nd Edn.; 2015
2. Organic Chemistry, R. T. Morrison and R. N. Boyd, S. K. Bhattacharjee. Pearson Education, 7th Edn.; 2014.
3. Medicinal Chemistry, Ashutosh Kar, New Age International, 3rd Edn.; 2005.
4. Fundamentals of Medicinal Chemistry, Gareth Thomas, Wiley Blackwell, 2003.
5. Organic Chemistry I. L. Finar Vol-II, ELBS Publications. 6th Edn.; 2002.

Semester-IV

M.Sc. SECOND YEAR
Forth Semester
Course Title: Natural Product and Medicinal Chemistry
Course code: PCH-CC-401

Credits = 4
M.M. = 100 (70+30)

Unit-I: Terpenoids

Isoprene rule, Classification, Nomenclature, General methods of structure determination, Stereochemistry and synthesis of α-Pinene, Menthol, farnesol and squalene. Biosynthetic routes to mono and sesquiterpenoids. Essential oils, their chemical composition, Extraction, Methods of analysis and their utility in flavour, Fragrance and pharmaceutical industries.

Unit-II: Flavonoids

Occurrence, Nomenclature and general methods of structure determination, Biosynthesis of flavonoids: Acetate pathway and shikimic acid pathway, Isolation and synthesis of Quercetin and Myrcetin, Bioactivity of flavonoids, anticancer, antioxidant and antibacterial activities of flavonoids.

Unit-III: Drug design

Drug Design: Classification and sources of drugs, concept of lead compounds and lead modification, Analogues, Prodrugs, Factors governing drug design, Structure activity relationship (SAR): isosterism, bioisosterism, changing the size and shape, Changing the number of methylene groups in chain, Changing the degree of unsaturation, Effect of introduction of methyl groups, Halogens, Hydroxyl, Carbonyl, Thiols sulphides groups and introduction/removal of ring systems on pharmacological activity.

Unit-IV: Antibiotics and anti-neoplastic drugs

Antibiotics: Classification, Cell wall biosynthesis, Inhibitors, β-lactam rings, Antibiotics inhibiting protein synthesis, Structure and synthesis of Pencillins, V & G chloroamphenical and tetracyclines, Anti-neoplastic drug: Introduction, cancer chemotherapy, plant derived anticancer agents, Taxol, Role of alkylating agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Books Recommended:

1. Mono and sesqueterpenoids, P. De-Mayo (Interscience-1959).
2. Terpene Chemistry, J. Verghese (Tata- Me GrawHill-1982).
3. Organic Chemistry, 5th Ed. Vol.2,1.L. Finar (Addison Wisley Longman-2000).
4. The Natural Pigment, Bentlay (Interscience).
5. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harwood Academic)
6. Introduction to Medicinal Chemistry Alex Gringauz (Wiley- VCH-1997).
7. Medicinal Chemistry- An Introduction, Gareth Thomas (Wiley-2000). 3rd Edition.
8. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
9. Medicinal Chemistry- V. K. Ahluwalia 2009, Ane Books Pvt.Ltd.
10. Gas-Chromatography- Mass Spectrometric Studies of Essential oils: An Analytical Approach, Manzoor Rather, Mushtaq Qurishi. (Lambert Academic Publishing-2011).

M.Sc. SECOND YEAR
Forth Semester
Course Title: Statistical Thermodynamics and Colloidal Chemistry
Course code: PCH-CC-402

Credits = 4
M.M. = 100 (70+30)

Unit I: Stastical Thermodynamics

Concept of Distribution, thermodynamic probability and most probable distribution, Sterling approximation, Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac distribution equations (without derivation).

Partition function and its significance, translational, rotational, vibrational and electronic partition function, Calculation of Thermodynamic properties in terms of partition functions, application to ideal monoatomic and diatomic gases, Equilibrium constant in terms of Partition Functions.

Unit-I: Canonical and Grand Canonical Ensembles

Concept of ensembles, ensemble average and postulate of equal a priori probability. Canonical, grand-canonical and Micro-canonical ensembles. Ensemble average. Perfect gas in canonical ensemble, Entropy and free energy. Grand canonical ensemble, Entropy and other thermodynamic functions in grand canonical ensemble.

Einstein model of Energy and heat capacity of a solid using canonical partition function. Limitations of Einstein model, Debye model of heat capacity.

Fluctuations and Real Gases: Mean of the distribution and the mean-square deviation, fluctuation in energy in a canonical ensemble.

Unit-III Surfactants, Micellar Solubilization and Catalysis

Classification of Surfactants, Solubility, Kraft temperature and cloud point, Micellization of surfactants; critical micelle concentration (cmc), aggregation number, Counterion binding, Factors affecting cmc in aqueous media. Thermodynamics of micellization: Pseudophase model and mass action models. Structure and shape of micelles: Geometrical consideration of chain packing, variation of micellar size and shape with surfactant concentration.

Solubilization, factors affecting micellar solubilization: nature of surfactant/solubilizate, effect of additive and temperature. Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release.
Micelles as reaction media: Theoretical consideration of reactions in micellar media, Examples of micellar catalysis for hydrolysis, Oxidation and reduction reactions.

Unit- IV: Block Copolymers and Polymer-Surfactant Mixtures

Block Copolymers: Introduction: classification, Micellization of diblock and triblock copolymers. Introduction to co-assembly of block copolymers by electrostatic interactions, Formation of polyion or block ionomer complexes, Introduction to pH-, thermo- and Photo-responsive block copolymers, Linear–dendrimer block copolymers: Introduction, Structural peculiarities of their aggregates, Potential applications.
Surfactant-Polymer Interactions: Effect of polymers on aggregation behavior of surfactants and the factors governing their interaction, Phase behavior of polymer-surfactant mixtures, Behavior of polyelectrolyte-surfactant systems, Technical applications of polymer surfactant systems.

Books suggested:

1. Norman Davidson, Statistical Mechanics, McGraw-Hill, New York.
2. R.P.H. Gasser and W.G. Richards, Introduction of Statistical Thermodynamics, World Scientific, Singapore (1995).
3. T.L. Hill, An Introduction to Statistical Thermodynamics, Dover, New York (1986).
4. Text book of physical chemistry, Atkins, MacQuarie.
5. D. Fennell Evans, H. Wennerstrom, ―The Colloidal Domain where physics, chemistry, biology and technology meet‖ VCH, New York, 1994.
6. Robert J. Hunter, ―Foundations of Colloid Science‖, Oxford University Press, New York, 2007.
7. P.C. Heimenz, ―Principles of Colloid and Surface Chemistry‖, Marcel Dekker Inc. New York, 1986.
8. M. J. Rosen, ―Surfactants and Interfacial Phenomena‖, John Wiley & Sons, New York, 2004.
9. R. D. Vold and M. J. Vold, ―Colloid and Interface Chemistry‖, Addison-wesley, 1982.
10. D. Y. Meyer, ―Surfaces, Interfaces and Colloid‖, VCH Publishers, Inc. 1991.
11. Jonsson, Lindmann, Homberg and Kronberg, ―Surfactants and polymers in aqueous solution‖, John Wiley and sons, 1998
12. Colloids and Interfaces with Surfactants and Polymers – An Introduction J. W. Goodwin, 2004, John Wiley & Sons Ltd, ISBN: 0-470-84142-7 (HB) ISBN: 0-470-84143-5 (PB).

13. FrederikWurm, Holger Frey: Linear–dendritic block copolymers: The state of the art and exciting, perspectives, *Progress in Polymer Science* 36 (2011) 1–52
14. M.J.Lawrence & G.D.Rees,Advanced Drug Delivery Reviews,Vol,45,p 898,2000.
15. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.

M.Sc. SECOND YEAR
Forth Semester
Course Title: Retro-Synthesis and Heterocyclic Chemistry
Course code: PCH-CC-403

Credits = 4
M.M. = 100 (70+30)

Unit-I: The Disconnection Approach:
An introduction to synthons and synthetic equivalents, The importance of order of events in organic synthesis, Functional group interconversions, The disconnection approach. One group, Two group and electrocyclic disconnections, Examples involving connections and rearrangements.
Protection of functional groups: Principle of protection of carbon-hydrogen bonds (in terminal alkynes and hydrogens of aldehydes), Carbon-carbon double bonds, Alcoholic hydroxyl groups, Amine groups, Carbonyl and carboxyl groups.

Unit-II: Carbon-Carbon (C-C) Disconnections:
One group C-C disconnections: alcohols and carbonyl compounds, Regioselectivity, Alkene Synthesis, Hydroboration and wittig reaction, Two group C-C disconnections: Diels Alder reaction, Michael addition and Robinson annulation, Examples of some illogical two group disconnections, Synthesis involving some illogical electrophiles.

Unit-III:

Nomenclature of monocyclic, Bicyclic and polycyclic heterocycles, Hantzsch-Widman nomenclature, Replacement nomenclature, Fusion nomenclature, Structure of five membered, six membered and bicyclic heteroatomic systems, Tautomerism in heterocyclic systems, Mesoionic systems, Criterion of aromaticity, Bond length, Resonance energy, Delocalization, UV/Visible and NMR spectroscopy of heterocycles.

Unit-IV:

Synthesis of aromatic heterocycles, Reaction types most frequently used in heterocyclic ring synthesis, Cyclisation reactions, Cycloaddition reactions, Electrocyclic processes in heterocyclic ring synthesis, Reactivity of aromatic heterocycles, Electrophilic addition at nitrogen, Electrophilic and nucleophilic substitution at carbon, De-protonation of N-Hydrogen.

Books Recommended:
1. Designing Organic Synthesis, S. Warren (Wiley-1978)
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin (Verlag VCH-1986).
3. Some Modern Methods of Organic Synthesis, 3rd Ed., W. Carruthers (Cambridge University Press-1986).
4. Modern Synthesis Reactions, 2nd Ed. H.O. House (W.A.Benjamin, NY-1972).
5. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 4th Ed., J. March, (Wiley-1992).
6. Principles of Organic Synthesis 2nd, R.O.C.Norman (Chapman and Hall-1978).
7. Heterocyclic Chemistry, 4th Ed., J.A.Joule and K. Mills (Black Well Science.
2000).
8. The Chemistry of Heterocycles: T. Eicher and S. Hauptman (Thieme-1995).

M.Sc. SECOND YEAR
Forth Semester
Course Title: Group Theory and Analytical Techniques
Course Code: PCH-CC-404

Credits = 4
M.M. = 100 (70+30)

Unit I: Symmetry Aspects of Molecular Vibrations

Introduction, the symmetry of normal vibrations, Determining the symmetry types of the normal modes (Normal mode analyses of water molecule, carbonate ion and N_2F_2), Contribution of particular internal coordinates to normal modes, Symmetry selection rules for fundamental vibrational transitions (qualitative treatment), The symmetry of group vibrations (a discussion of molecule $Cl_3C\text{-}CH_2\text{-}CCl_3$ to demonstrate vibrational modes of CH_2 group). Use of symmetry considerations to determine the number of active infrared and raman lines (example SF_4).

Unit II: Symmetry Aspects of Hybrid Orbitals

Transformations properties of atomic orbitals. Hybrid orbitals for sigma bonds in trigonal planar (BCl_3), Tetrahedral (CH_4), Square planar $[PtCl_4]^2$ - and trigonal bipyramidal (PF_5), Hybridization scheme for pi bonding in trigonal planar (AB_3) and tetrahedral (AB_4) systems, Mathematical form of equivalent and non-equivalent hybrid orbitals, Trigonal planar sp^2 equivalent hybrids in BCl_3; Tetrahedral sp^3 equivalent hybrid orbitals in CH_4 and trigonal bipyramidal dsp^3 non-equivalent hybrid orbitals in PF_5.

Unit-IV: Thermal Methods of Analysis
Thermo gravimetric analysis (TGA), Apparatus, Methodology, Applications of TGA for quantitative analysis (TG analysis of CaC_2O_4. H_2O, $CuSO_4$. $5H_2O$, dolomite ore, etc.) and problems based TGA.
Differential thermal analysis (DTA), Apparatus, Methodology, Application, Comparative study of TGA and DTA, Interpretation of TGA and DTA curves of important compounds e.g., Calcium oxalate monohydrate, Magnesium oxalate monohydrate, Analysis of silver-copper alloy and dolomite sample by TGA.
Thermometric titrimetry and applications to acid-base and complexometric titrations.

Unit IV: Polarography and voltammetry

Polarographic principles, the dropping mercury electrode (DME), diffusion current, factors affecting the diffusion current, dependence of 'm' upon mercury height, effect of temperature, limiting current and residual current, potential range of the DME, interfering electrode reactions, polarographic maxima, Ilkovic equation, polarographic analysis, interpretation of polarographic wave equation, AC polarography, pulse polarography, differential pulse polarography, linear sweep and cyclic voltammetry

Books Recommended

1. Chemical Applications of Group Theory: by F.A. Cotton.
2. Group Theory and Symmetry in Chemistry: by Lowell H. Hall.
3. Symmetry, Orbitals and Spectra: by Milton Orchin and H.H. Jaffe.
4. Physical Methods in Chemistry: by R.S. Drago. 5. Molecular Spectroscopy: by G.M. Barrow, McGraw-Hill.
5. Ionic Equilibria in Analytical Chemistry; Freiser and Fernando.
6. Introduction to chemical Analysis, R. D.Braun, Mc. Graw-Hill, International Book Co., 1983
7. Chemical Analysis, 2nd Ed., H.A. Laitinen and W.E. Harris, McGraw Hill Kogakusha, Ltd., 1975.
8. Instrumental Methods of Analysis, 7th Ed., Willard, Merritt, Dean and Settle, CBS Publishers, New Delhi.
9. Instrumental methods of Chemical Analysis, 5th edn., G.W. Ewig, McGraw Hill Book Co., 1985.
10. Instrumental Methods of Analysis by G.D. Christian and C.N. Reilly.
11. Principle of Instrumental Methods of Analysis; D.A. Skoog. D.M. West and F.J. Holler, Sounders College Publishing New York, 2001.

Syllabus
for
(Open Elective Course)

Open Elective Course

Course Title: Surfactants, Soaps, and Detergents

Course Code: PCH-OE-401

Credits =2

M.M. = 50 (35+15)

Unit-I: Surfactants

Classification and micellization of surfactants: critical micelle concentration (CMC), aggregation number, Counterion dissociation and binding, Factors affecting CMC in aqueous media. Solubility of surfactants, Kraft temperature and cloud point, Properties of solutions of surface Active Agents, Driving force for micelle Formation, Surfactants in personal Care products and Cosmetics, Introduction to Lotions, Hand Creams, Lipsticks, Nail polish, Shampoos, Antiperspirants, Foundations, Surfactants used in cosmetic formulations.

Unit-II: Soaps and Detergents

Mechanism of cleansing soaps, Action of soap, Effect of the alkali, Effects of fats, Liquid soap, Soap-making processes, Cold process, Hot processes, Molds, Purification and finishing. Chemical classification of detergents, Anionic detergents, Cationic detergents, Non-ionic and zwitterionic detergents. Major applications of detergents, Laundry detergents, Fuel additives, Biological reagent, Soapless soap.

Books Recommended:

1. Applied Surfactants: Principles and Applications; T. F. Tadros, Wiley-Vch Verlag GmbH and Co. KGaA, 2005.
2. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
3. Physical Chemistry; P.W. Atkins; ELBS; Oxford; 1994.
4. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
5. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York.; 1986.
6. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley.; 1982.