Syllabus of M.Sc. in Chemistry

JIS UNIVERSITY,
81, Nilgunj Road, Agarpara,
Kolkata-700109

JIS UNIVERSITY, KOLKATA

M.Sc. in Chemistry

FIRST SEMESTER

Sl. No.	Course Code	SUBJECT	PERIODS			CREDIT
			L	T	P	
THEORY						
1	MCH-101	Analytical Chemistry I	3	1	0	4
2	MCH-102	Inorganic Chemistry I	3	1	0	4
3	MCH-103	Organic Chemistry I	3	1	0	4
4	MCH-104	Physical Chemistry I	3	1	0	4
Practical						
5	MCH-191	Inorganic Chemistry Lab I	0	0	3	2
6	MCH-192	Organic Chemistry Lab I	0	0	3	2
7	MCH-193	Physical Chemistry Lab I	0	0	3	2
8	MSD-181	Project & Seminar	0	0	0	1
Total			12	4	9	23

JIS UNIVERSITY, KOLKATA

M.Sc. in Chemistry

SECOND SEMESTER

Sl. No.	Course Code	SUBJECT	PERIODS			CREDIT
			L	T	P	
THEORY						
1	MCH-201	Analytical Chemistry II	3	1	0	4
2	MCH-202	Inorganic Chemistry II	3	1	0	4
3	MCH-203	Organic Chemistry II	3	1	0	4
4	MCH-204	Physical Chemistry II	3	1	0	4
5	MCS-201	Computer Applications in Physics and Chemistry	3	0	2	4
PRACTICAL						
6	MCH-291	Inorganic Chemistry Lab II	0	0	3	2
7	MCH-292	Organic Chemistry Lab II	0	0	3	2
8	MCH-293	Physical Chemistry Lab II	0	0	3	2
9	MSD-281	Project & Seminar	0	0	0	1
10	MSD-282	Skill Development	0	0	0	1
Total			15	4	11	28

JIS UNIVERSITY, KOLKATA

M.Sc. in Chemistry

THIRD SEMESTER

Sl. No.	Course Code	SUBJECT	PERIODS			CREDIT
			L	T	P	
THEORY						
1	MCH-301	Principles and Applications of Molecular Spectroscopy	3	1	0	4
2	MCH-302	Biological Chemistry	3	1	0	4
3	MCH-303/304/305	Special Paper I (Inorganic/Organic/Physical)	3	1	0	4
4	MCH-306/307/308	Special Paper II (Inorganic/Organic/Physical)	3	1	0	4
5	MCH-309/310	Elective I	3	0	0	3
PRACTICAL						
6	MCH-391/392/393	Inorganic/Organic/Physical Chemistry Lab III	0	0	9	6
7	MSD-381	Project & Seminar	0	0	0	1
Total			15	4	9	26

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FOURTH SEMESTER

Sl. No.	Course Code	SUBJECT	PERIODS			CREDIT
			L	T	P	
THEORY						
1	MCH-401	Spectroscopy for Structure Elucidation	3	1	0	4
2	MCH-402	Polymer and Materials Chemistry	3	1	0	4
3	MCH-403/404/405	Special Paper III (Inorganic/Organic/Physical)	3	0	0	3
4	MCH-406/407/408	Special Paper IV (Inorganic/Organic/Physical)	3	0	0	3
5	MCH-409/410	Elective II	3	0	0	3
PRACTICAL						
6	MCHD-491	PROJECT	0	0	12	8
7	MSD-481	Project & Seminar	0	0	0	1
8	MSD-482	Skill Development	0	0	0	1
Total			15	2	12	27

Semester III

Specialization Paper I

MCH-303: Advanced Bioinorganic and Organometallics
MCH-304: Advanced Organic Synthesis I
MCH-305: Advanced Quantum Mechanics

Specialization Paper II

MCH-306: Advanced Topics in Inorganic Chemistry I
MCH-307: Pericyclic and Photochemistry
MCH-308: Solid State Chemistry

Elective paper I
MCH-309: Supramolecular Chemistry & Drug Design
MCH-310: Nuclear Chemistry

Semester IV

Specialization Paper III

MCH-403: Inorganic Reaction Mechanism & Photochemistry
MCH-404: Advanced Organic Synthesis II
MCH-405: Electrochemistry

Specialization Paper IV

MCH-406: Advanced Topics in Inorganic Chemistry II
MCH-407: Heterocyclic Chemistry
MCH-408: Statistical Mechanics

Elective paper II
MCH-409: Chemical Applications of Group Theory
MCH-410: Advanced Spectroscopy

Detailed Syllabus of First semester

MCH-101: Analytical Chemistry I

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Introduction

Scope and objectives, classification of analytical methods, method selection, sample processing, steps in a quantitative analysis, quantitative range, data organisation, analytical validations, limit of detection and quantification, tools of analytical chemistry and good lab practices.

Unit-2: Separation techniques

Solvent extraction: principle, distribution ratio and partition coefficient, successive extraction and separation, different methods of extraction systems, Craig extraction and counter current distribution, problems.

Chromatography: general principle, classification, mathematical relations of capacity, selectivity factor, distribution constant and retention time, chromatogram, elution in column chromatography: band broadening and column efficiency, van Deemter equation, column resolution, numerical problems, gas chromatography, high performance chromatography and supercritical fluid chromatography: principles, methods, comparison and applications, thin-layer chromatography, size-exclusion chromatography, ion chromatography and capillary electrophoresis: principles, methods and applications.

Unit-3: Environmental chemistry

Introduction: environmental segments, atmospheric structure chemistry of lower and upper atmosphere, radiation balance of earth.

Air pollution: major air pollutant, air quality standards and norms, determination of air pollutants, Greenhouse effect, mechanistic pathways of smog formation and ozone hole, acid rain, global warming, technology of air pollution abatement.

Water pollution: classification of water pollutants, characteristics of waste water, water quality parameters and their measurements, biochemical effects of As, Pb, Cd, Hg and their chemical speciation, eutrophication, waste water treatment: preliminary, primary, secondary, tertiary treatment.

Solid waste disposal and management: classification and origin, methods of solid waste disposal, microbiology involved in solid waste disposal.

Soil pollution: chemical composition of the soil, the exploitation of the mineral resources and abuse of the earth, soil pollution due to natural and artificial agencies and its effects, remedial measures to check the pollution.

Energy and Environment: energy sources, renewable and non-renewable, primary and secondary fossil fuels, their occurrence and estimation.

Recommended Books

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
2. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.
3. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry - An Introduction, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
4. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.
5. Mani Vasakam, Physico Chemical Examination of Water, Sewage and Industrial effluents, Pragati Prakashan, 1991
6. F. W. Fifield and W. P. J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.
7. Colin Baird, Environmental Chemistry, W. H. Freeman and Company, New York (1995).
8. A. K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
9. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.
10. S. M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
11. S. K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

MCH-102: Inorganic Chemistry I

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Lanthanides and Actinides

Lanthanides and Actinides, extraction, properties, redox chemistry, general characteristics, spectral and magnetic properties.

Unit-2: Quantum mechanical approach to Chemical bonding

LCAO-MO and Huckel approximation to H_2^+, H_2, homo and hetero diatomic, triatomic and polyatomic molecules/ions, application of V.B. and M.O. theories to diatomic and polyatomic molecules.

Unit-3: Coordination chemistry and Electronic spectra

Crystal field theory, crystal field diagram, concept of CFSE and OSPE and their applications, Jahn-Teller distortions, Spectrochemical and Nephelauxetic series, thermodynamic, structural, and kinetic aspects of CFT, ligand field theory, molecular orbital theory and angular overlap model.

Electronic spectral properties of transition metal complexes: microstates, determination of spectroscopic ground state/term symbols, Orgel and Tanabe-Sugano diagrams, selection rules for spectral transition, d-d spectra, charge transfer spectra and calculation of crystal field parameters.

Recommended Books

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John Wiley & Sons, New York.
2. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principles of structure and reactivity, Harper Collins 1993.
3. R. S. Drago, Physical Methods in Inorganic Chemistry, International Edn. (1971), Affiliated East-West Press, New Delhi.
4. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, W. B. Sauders Com. (1987), Hong Kong.
5. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International Pvt. Ltd., New Delhi (1999).
6. B.N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd. New Delhi (1976).
7. D. J. Newman, Betty, Crystal Field, Science, 2000
8. M. Chanda, Structure and Chemical bond, Tata McGraw Hill Atomic Edition, 2000.
9. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford University Press, 1990.

MCH-103: Organic Chemistry I

L-T-P: 3-1-0 **Credit: 4**

Unit 1: Reaction mechanism I

Concise review on nucleophilic, electrophilic substitution reactions, and elimination reactions, neighbouring group participation: the phenonium ion, participation by π and σ bonds, Anchimeric assistance, classical versus non-classical carbonium ions- the present status.

Unit 2: Aromaticity

Huckel's rule, concept of aromaticity in benzenoid and nonbenzenoid systems, alternate and non-alternante hydrocarbons, annulenes, heteroannulenes, fullerenes, anti-aromaticity, pseudo-aromaticity, homo-aromaticity.

Unit 3: Structural effects on reactivity

Linear free energy relationships (LFER), the Hammett equation, substitutent constants, theories of substitutent effects, interpretation of σ-values, reaction constant ρ, deviations from Hammett equation, dual - parameter correlations, inductive substituent constant, the Taft equation.

Unit 4: Stereochemistry

Molecular symmetry, chirality, point groups, stereoisomerism, configuration: relative and absolute, determination of relative configuration: Prelog's rule, Cram's rule, and Sharpless rule, *conformation:* conformational analysis of acyclic, cyclic, fused, spiro and bridged bicyclo-systems with typical examples.

Recommended Books

1. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2001.
2. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
3. Peter Sykes, A Guide book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.
4. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, Ist Edition (1990), Macmillan India Ltd., New Delhi.
5. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi.
6. E.L. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Organic Compounds, Wiley Interscience, New York (2004).

MCH-104: Physical Chemistry I

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Thermodynamics

Concise review of thermodynamics, concept of partial molar quantities and their significances, Nernst heat theorem, consequences of Nernst heat theorem, entropy and third law of thermodynamics: determination of absolute entropy, concept and significance of residual entropy.

Thermodynamic probability and entropy, distribution laws: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac, concept of partition function: rotational, translational, vibrational and electronic partition functions of diatomic molecules, concept of ensembles, relation between partition functions with various thermodynamic functions, Gibb's paradox.

Unit-2: Chemical kinetics

Concise review of chemical kinetics, fast reactions: luminescence and energy transfer processes, kinetics study of fast reactions by stopped–flow and relaxation, and flash photolysis methods.

Rate equations of photochemical, chain and oscillatory reactions, thermodynamic treatment of transition state theory, theories of unimolecular reactions: Lindemann-Christiansen hypothesis, Hinshelwood, Rice-Ramsperger- Kassel (RRK), and Rice- Ramsperger-Kassel-Marcus (RRKM).

Unit-3: Surface chemistry

Adsorption: different types of adsorption, absorption vs adsorption, different adsorption isotherms, unimolecular and bimolecular surface reaction, activation energy of such reactions, volcano curve.

Transition state theory of surface reactions: rates of chemisorptions and desorption, unimolecular and bimolecular surface reaction.

Micelles: Surface active agents and their classifications, micellization, factors affecting cmc of surfactants. Thermodynamics of micellization: phase separation and mass action models. Emulsions and reverse micelle.

Recommended Books

1. G.W. Castellan, Physical Chemistry, 3rd Edition, Narosa Publishing House
2. P.W. Atkins, Physical Chemistry, 8th Editions, Oxford University Press, New York
3. K.J. Lailder, Chemical Kinetics, 3rd Edition, Pearson
4. I.N. Levine, Physical Chemistry, 5th Edition, Tata McGraw Hill Publication Co, Ltd, New Delhi
5. B.K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi
6. D.A. Mcquarrie, Statistical Mechanics, California University Science Books
7. R. K. Patharia, Statistical Mechanics, Butterworth, Heinemann, Elsevier
8. Y. Moroi, Micelles: Theoretical and Applied Aspects, Plenum Press, New York (1992)
9. T. Engel, P. Reid, Thermodynamics, Statistical thermodynamics and Kinetics, Pearson
10. E. S. R. Gopal, Statistical Mechanics and Properties of Matter, Ellis Horwood, England, 1974.

MCH-191: Inorganic Chemistry Lab I

L-T-P: 0-0-3 **Credit: 2**

- Quantitative analysis of metal ions in binary mixture by complexometric titrations
- Synthesis and characterization of different coordination complexes
- Separation and estimation of binary mixtures by ion-exchange method
- Separation of cations or anions in a mixture by paper chromatography

MCH-192: Organic Chemistry Lab I

L-T-P: 0-0-3 **Credit: 2**

- Detection and identification of organic compounds through chemical test, UV and IR
- Organic synthesis: Nitration, Bromination, Condensation, Reduction and Hydrolysis involving at least two steps

MCH-193: Physical Chemistry Lab I

L-T-P: 0-0-3 **Credit: 2**

- Determination of specific rate constant of acid catalyzed hydrolysis of ester at two different temperature and evaluate the corresponding thermodynamic parameters
- Compare the strength of acids (HCl vs H_2SO_4) by studying the hydrolysis of ester
- Evaluate the energy of activation for saponification of ester
- Determination of rate constant of acid catalyzed hydrolysis of sucrose by a polarimeter
- To construct the phase diagram of three component systems
- Determination of heat of solution of oxalic acid from its solubility at different temperature
- Determination of isoelectric point
- Verification of adsorption isotherm by adsorption of acetic acid on charcoal
- Any other experiments related to thermodynamics, kinetics, adsorption and micelle performed in the laboratory during the semester

Recommended Books

1. A.I. Vogel, A Textbook of Quantitative Inorganic Analysis, ELBS
2. Ghosal, Mahaparta and Nad, An Advanced Course in Practical chemistry
3. G. N. Mukherjee, Handbook of Practical Chemistry
4. A.I. Vogel, A Textbook of Practical Organic Chemistry
5. A. M. James, F. F. Prichard, Practical Physical Chemistry
6. Shoermaker, Garland, Experimental Physical Chemistry

Detailed Syllabus of Second semester

MCH-201: Analytical Chemistry II

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Spectroscopic techniques

Theory, instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), atomic absorption spectroscopy, atomic fluorescence spectrometry, atomic emission spectrometry, inductively coupled plasma-atomic absorption spectrometry.

Unit-2: Electroanalytical methods

Theory, instrumentation and applications of voltammetry, linear sweep voltammetry, anodic stripping voltammetry, cyclic voltammetry, amperometry, coulometry, electrogravimetry and polarography: electrochemical cell, reference and indicator electrodes, membrane electrodes, electrode-solution interface layer, electrolytic process, DME, Cottrell equation, Ilkovic equation, half wave potential and its significance, test of reversibility, current-voltage diagram.

Unit-3: Thermal methods

Theory, methodology and applications of thermogravimetric analysis (TGA), differential thermal analysis (DTA), and differential scanning calorimetry (DSC), thermal stability of covalent and non-covalent bonds, thermal degradation, single crystal phase transformation, thermochemiluminescence, thermometric titration, solid state reaction kinetics.

Recommended Books

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
2. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.
3. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College of Publishing, Philadelphia, London.
4. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry - An Introduction, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
5. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.
6. A. J. Bard, Electroanalytical Chemistry
7. J. W. Robinson, Atomic absorption Spectrometry
8. D. A. Skoog, D.M. West, F.J. Holler, Fundamentals of Analytical Chemistry
9. H. H. Willard, L. L. Meritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis
10. H.A. Strobel, Chemical Instrumentation: A Schematic Approach, 2nd Edition (1973)

MCH-202: Inorganic Chemistry II

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Elements of group theory

Groups, subgroups, classes and characters, classes of symmetry operations, symmetry points groups: representation of groups by matrices, representation of symmetry operator-tranformation of basis vector, symmetry transformation of operators, the great orthogonality theorem and its consequences, construction and application of character table.

Unit-2: Organometallic Chemistry I

Application of 18- electron and 16- electron rules to transition metal organometallics, structure, bonding (pictorial mo-approach) and reactions of η^2-ethylinic, η^3-allylic and η^5-cyclo-pentadineyl compounds, structure and bonding of carbonyls, nitrosyls and related pi- acids, alkyl, alkene, alkyne, π-allyl, polyene and cyclopolyene compounds; metal carbenes and carbynes, isolobal analogy, Dewar-Chatt model, oxophilicity, Agostic interaction, organo-metallic catalysts.

Unit-3: Bioinorganic Chemistry I

The roles of metal ions in biological process, Ion transport across biological membrane and its significance, mechanism of Na^+/K^+-ion pump; Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin, model synthetic dioxygen complexes.

Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (ferredoxines). cytochrome c oxidase.

Recommended Books

1. F. A. Cotton, Chemical Applications of Group Theory
2. R. H. Crabtree, The Organometallic Chemistry of Transition Metals
3. B.D.Gupta and A.J. Elias, Basic Organometalltic Chemistry
4. I. Bertini, H. B. Grey, S. J. Lippard, J. S. Valentine, Bioinorganic Chemistry
5. Asim K. Das, Bioinorganic Chemistry

MCH-203: Organic Chemistry II

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Reaction mechanism II

Addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity, hydrogenation, hydroboration reaction.

Addition to carbon-hetero multiple bonds: mechanism of metal hydride reaction of substituted and unsubstituted carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organocopper, organozinc, organolithium and organosilane reagents to saturated and unsaturated carbonyl compounds.

Unit-2: Organic Name reaction

Birch reduction, Aldol condensation, Wittig reaction, Simmons-Smith cyclopropanation, Nef reaction, Favorskii reaction, Baeyer-Villiger oxidation, Claisen rearrangement, Beckmann rearrangement, Shapiro reaction, Mitsunobu reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, Ene reaction, Mannich reaction, Stork enamine reaction, Michael addition, Robinson annulation, Barton decarboxylation and deoxygenation reaction, Sharpless asymmetric epoxidation, Norrish type-I & II reaction, di-pi methane rearrangement, paterno-Buchi reaction.

Unit-3: Reagents and Reactions

(i) Gilman's reagent–Lithium dimethylcuprate, (ii) Lithium diisopropylamide (LDA), (iii) Dicyclohexyl carbodiimide (DDC), (iv) 1,3-Dithiane (Umpolung reagent), (v) Peterson's synthesis, (vi) Bakers yeast, (vii) DDQ, (viii) Palladium catalysed reactions, (ix) Woodward and Prevost hydroxylation, (x) Iodotrimethyl silane.

Unit-4: Natural Products I

Biosynthesis of (i) Non-nitrogenous secondary metabolites from Shikinic acid, flavonoids and related polyphenolics, (ii) mono- and di-terpenoids from Mevalonic acid (iii) tri-terpenoids from geranyl pyrophosphate.

Recommended Books

1. Clayden, Greeves, Warren, Organic Chemistry
2. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry
3. W. Carruthers, I. Coldham, Modern method of Organic Synthesis
4. Michael B. Smith, Jerry March, March's Advanced Organic Chemistry. Reactions, Mechanisms, and Structure
5. Jie Jack Li , Name Reactions: A Collection of Detailed Reaction Mechanisms
6. Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, Name Reactions and Reagents in Organic Synthesis
7. I. L. Finar, Organic Chemistry (Volume 1 & 2)

MCH-204: Physical Chemistry II

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Quantum Mechanics

Origin of quantum mechanics, Black-body radiation, photoelectric effect, Compton effect, Pair production, de Broglie's hypothesis: Davisson-Germer's and Thomson's experiment, Wave-particle duality: Franck-Hertz experiment, Young's double slit experiment, Heisenberg's uncertainty principle.

Operators, Eigen functions, Hermitian operator, Postulates of quantum mechanics, Angular momentum, its commutative relations, Ladder operator, Pauli spin operator, Schrodinger wave equation and its formulation as an eigen value problem.

Translational motion of a particle, particle in one, two and three dimensional boxes, harmonic-oscillator, rotational motion of a particle: particle on a ring, particle on a sphere, rigid rotator, step-potential, tunneling, hydrogen atom.

Introduction to approximation methods: Perturbation theory and Variational method.

Unit-2: Electrochemistry

Quantitative treatment of Debye-Hückel theory of ion-ion interaction, its applications and limitations, modification of Debye-Hückel law for finite-sized ions, Debye-Hückel-Onsagar equation, association of ions: Bjerrum and Fuoss model, electrode kinetics, current-overpotential relationship, Tafel equation and its importance.

Recommended Books

1. I. N. Levine, Quantum Chemistry, 5th Edition (2000), Pearson Educ., Inc. New Delhi
2. Donald A McQuarrie, Quantum Chemistry, Viva Student Edition, Viva Books, NewDelhi
3. D. J. Grffiths, Introduction to Quantum Mechanics
4. J. L. Powell, B. Crasemann, Quantum Mechanics
5. D. A. McQuarrie, J. D. Simon, Physical Chemistry, A Molecular Approach, (1998), Viva Books, New Delhi
6. Richard L. Liboff, Introductory Quantum Mechanics
7. R.K. Prasad, Quantum Mechanics
8. Samuel Glasstone, An Introduction To Electrochemistry, Affiliated East-West Press Pvt. Ltd.-New Delhi (2000)
9. J. O'M. Bockris, A. K. N. Reddy, Modern Electrochemistry, Vol. 2 A & B, 2nd Edition, Plenum Press, New York (1998)

MCH-291: Inorganic Chemistry Lab II

L-T-P: 0-0-3 **Credit: 2**

- Qualitative analysis of mixture of compounds containing six radicals of which two are rare elements
- Tritrimetric estimation of mixtures of metal ions by EDTA
- Spectroscopic estimation of inorganic complexes
- Job's method of continuous variation

MCH-292: Organic Chemistry Lab II

L-T-P: 0-0-3 **Credit: 2**

- Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components
- Small scale organic synthesis by exploiting common organic reactions and their purification

MCH-293: Physical Chemistry Lab II

L-T-P: 0-0-3 **Credit: 2**

- Determination of rate constant of alkaline hydrolysis of ester conductometrically
- Conductometric titration of mixture of acids (HCl and CH_3CO_2H)
- Determination of the individual strengths of $(NH_4)_2SO_4$ and Na_2SO_4 in a mixture conductometrically
- Conductometric titration of Zn(II) vs $K_4[Fe(CN)_6]$ and determination of composition of the complex
- Determination of CMC of SDS conductometrically
- Potentiometric titration of mixture of acids (HCl and CH_3CO_2H)
- Determination of the formal redox potential of $Fe^{2+/}Fe^{3+}$ system potentiometrically
- Potentiometric titration of $K_4[Fe(CN)_6]$ by $ZnSO_4$ or $Pb(NO_3)_2$ and determination of composition of the complex
- Verification of Lambert and Beer's law. Also determine the concentration of an unknown solution from calibration curve
- Determination of pKin of bromocresol green indicator

Recommended Books

1. A.I. Vogel, Qualitative Inorganic Analysis
2. A.I. Vogel, A Textbook of Quantitative Inorganic Analysis, ELBS
3. Ghosal, Mahaparta and Nad, An Advanced Course in Practical chemistry
4. G. N. Mukherjee, Handbook of Practical Chemistry
5. A.I. Vogel, A Textbook of Practical Organic Chemistry
6. A. M. James, F. F. Prichard, Practical Physical Chemistry
7. Shoermaker, Garland, Experimental Physical Chemistry

Detailed Syllabus of Third semester

MCH-301: Principles and Applications of Molecular Spectroscopy

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Fundamentals

Interaction of electromagnetic radiation with matter, Einstein coefficient, transition probability, transition dipole moments and selection rules, intensity of spectral lines, line-widths and line shapes, Fourier transforms in spectroscopy.

Unit-2: Rotational and Vibrational spectroscopy

Classifications of molecules based on topicity, microwave and vibrational spectroscopy of diatomic and polyatomic molecules, energy levels, selection rules, isotope effect, non-rigidity on spectral features, vibration and group frequency, vibration-rotation spectra of diatomic molecules, origin of P, Q, and R branch, hot bands, applications.

Unit-3: Raman spectroscopy

Raman spectra of diatomic molecules, rotational and rotation- vibrational Raman transitions, effects of nuclear spin, polarization of Raman lines, applications.

Unit-4: Electronic spectroscopy

Origin, selection rules, spectral features, Franck-Condon principle, dissociation and pre-dissociation, rotational fine structure, charge transfer spectra, fluorescence and phosphorescence spectra, applications.

Unit-5: LASER spectroscopy

General features, principles, characteristics of laser, population inversion, basic elements in laser pulsed, lasers, laser cavity modes, Q-switching, mode locking, harmonic generation, different lasers: He-Ne, Nd-YAG, titanium-sapphire, dye lasers, semiconductor lasers, and applications of lasers in spectroscopy.

Unit-6: Photoelectron Spectroscopy

Photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS of simple molecules, applications.

Unit-7: Nuclear Magnetic resonance spectroscopy

Basic principles, relaxation times, intensity of NMR signals, electronic shielding, NMR in liquids: chemical shifts, origin of spin-spin couplings, and qualitative idea about NMR spectra of AX, AX_2, A_3X and AB systems.

FT-NMR: Rotating frame of reference, effect of radiofrequency pulses, FID, Multi pulse operation, measurement of T_1 by inversion recovery method, spin echo and measurement of T_2.

Recommended Books

1. J. M. Hollas, Modern Spectroscopy, 4th edition (2004) John Wiley & Sons, Ltd., Chichester.
2. C. N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.
3. J. D. Graybeal, Molecular spectroscopy
4. I. N. Levine, Molecular spectroscopy
5. G. Herzburg, Infrared and Raman Spectra (1945), Spectra of Diatomic Molecules (1950), Van Nostrand, New York.
6. J. R. Lakowicz, Principles of Fluorescence Spectroscopy
7. W. Demtroder, Laser Spectroscopy
8. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill International Book Company, Tokyo, 1982.
9. R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, (1986) Addison Wesley, Longman Ltd, London.
10. A Carrington and A. D. Mc Lachlan, Introduction to Magnetic Resonance, (1979) Chapman and Hall, London.

MCH-302: Biological Chemistry

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Proteins and Nucleic Acids

Natural and synthetic amino acids, different synthetic strategy of peptides, structure and function of protein and nucleic acids, Ramachandran plot, denaturation of proteins, factors affecting denaturation, structural aspect of protein with respect to haemglobulin and myoglobulin, protein folding, doble helical structure of DNA, RNA, various forms of DNA (a, b, c, z) and RNA (m& t), transcription and translation, gene expression, DNA binding protein-zinc-finger protein, and oxygen uptake proteins: Hemerythrin and Hemocyanin.

Unit-2: Enzymes, Carbohydrates, Lipids, Hormones and Steroids

Classification, function and regulation of enzymes, active sites, Vitamins as coenzymes and co-factors, enzyme kinetics, TON and TOF, enzyme inhibitors, structure and function of Carbonic anhydrase, Superoxide dismutase, Urease, Hydrogenase, and Carboxy-peptidase etc. Structure, function and reactions of carbohydrates, lipids, hormones and steroids; Epinephrine, Norepinephrine, Cholesterol, Prostaglandins, and cell membranes.

Unit-3: Bioenergetics

Glycolysis, citric acid cycle, electron transport chain, oxidative phosphorylation, membrane transport mechanism.

Recommended Books

1. L. Stryer, Biochemistry, 5th edition (2002), Freeman & Co., New York.
2. D. L. Nelson and M. M. Cox, Lehninger, Principles of Biochemistry, 3rd edition (2002) McMillan North Publication.
3. M. N. Hughes, Inorganic Chemistry of Biological Processes, (1981) John Wiley.
4. M. B. Smith, Organic Synthesis, (1995) McGraw Hill Inc., New York.
5. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.

MCH-303: Advanced Bioinorganic and Organometallics

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Bioinorganic Chemistry II

Role of alkaline earth metal ions in biological systems: (i) Catalysis of phosphate transfer by Mg^{2+} ion, (ii) Ubiquitous regulatory role of Ca^{2+} in muscle contraction

Metalloenzymes: catalase, peroxidise, SOD, cytochrome-450, NOS, Urease, Hydrogenase. Biological and abiological nitrogen fixing systems. Molybdo enzymes: nitrate reductases, sulfite oxidase.

Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water, model systems.

Bioinorganic chemistry of human iron metabolism: ferritin and transferin.

Vitamins and coenzymes: Vitamin B6 and vitamin B12 coenzymes, model systems.

Toxicity and drugs: Toxic effects of metal ions, detoxification by chelation therapy, metal dependent diseases and metal complexes as drugs, Pt, Ru, Rh and Au drugs.

Unit-2: Organometallic Chemistry II

Complexes of π and σ-donor ligands: Complexes of dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands, transition metal alkenyls, alkynyls, carbenes and carbines.

π-complexes of unsaturated molecules: Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

Metal-metal single and multiple bonding (pictorial MO–approach), bond orders, bonding in direhnium compounds, Isolobal and Isoelectronic relationships.

Transition metal complexes in catalysis: Hydrogenation, hydroformylation, polymerization, and Waker process.

Recommended Books

1. M. N. Hughes, Inorganic Chemistry of Biological Processes, 2nd Ed.(1981), John-Wiley & Sons, New York.
2. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York (1995).
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).
4. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi (1998)
5. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed. (1999) John Wiley & Sons.
6. J. E. Huheey, Keiter and Keiter, Inorganic Chemistry.
7. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, John Wiley.
8. Ch. Elschenbroich and A. Salzer, Organometallics, VCH.
9. J. P. Collman, L. S. Hegedus, J. R. Norton and R.G. Finke, Principles and Applications of Organotransition metal Chemistry, Univ. Sci. Books, Mill Valley. California.

MCH-304: Advanced Organic Synthesis I

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Radical reaction in Organic Chemistry

Definition, generation of free radicals, detection, shapes and stability, stable free radicals. Example of addition, substitution, oxidation, cyclization and rearrangement involving radical reaction mechanism.

Unit-2: Protection and Deprotection

The role of protective groups in organic synthesis, principle of protection and deprotection, Different procedure for protection and deprotection of hydroxyl (including 1,2- and 1,3-dihydroxy), phenols, amines, carbonyls and carboxylic groups.

Unit-3: Redox reactions in Organic synthesis

Fundamentals, *Oxidation of alcohols:* By Chromium and Manganese reagents, Silver carbonate, oxidation via alkoxysulphonium salts and other methods. *Oxidation of Carbon-Carbon double bonds:* dihydroxylation, diastereoselective epoxidation of homoallylic alcohols, photosensitized oxidation of alkenes, Pd-catalyzed oxidation of alkenes, use of Ruthenium tetroxide and Thallium (III) nitrate as oxidizing agents for organic substrate, other oxidizing agents. *Reduction by dissolving Metals*: reduction with metal and acid (reduction of carbonyl compounds), desulphurisation of thio-acetals, reduction of organic compounds by di-imide, lowvalent Titanium reagents, trialkyltin hydrides, trialkylsilanes and other reagents.

Unit-4: Natural Products II

Structure and stereochemistry of alkaloids (Atropine/ Quinine); Terpenoids (Abietic acid/ β-Carotene); Steroids (Cholesterol). Biosynthesis of Atropine, Quinine, Abietic acid, β-Carotene, Cholesterol.

Recommended Books

1. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2001.
2. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
3. Peter Sykes, A Guide book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient Longman Ltd., New Delhi.
4. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, Ist Edition (1990), Macmillan India Ltd., New Delhi.
5. F.A. Carey and R.J. Sundburg,, Advanced Organic Chemistry, Part-A
6. F.A. Carey and R.J. Sundburg, Advanced Organic Chemistry, Part-B

MCH-305: Advanced Quantum Mechanics

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Fundamental principles

Postulates of quantum mechanics, Schmidt orthonormalisation, Fourier transformation, delta function with examples, tunneling, bound states, the Virial theorem.

Unit-2: Approximation methods in quantum mechanics

Stationary perturbation theory for non-degenerate and degenerate systems and its applications to rotator, Stark effect, the Helium atom, Variation method, principles of linear and non-linear variation methods and its applications, JWKB approximation, time-dependent perturbation theory, radiative transitions, transition probability and rates, Einstein coefficients, selection rules.

Unit-3: Quantum mechanics of many electron atoms

Pauli's antisymmetry principle, antisymmetry of many electron wave function, spin and spatial orbitals, Slater determinant, closed-shell and open-shell electron configurations, multi-electron pure-spin state wave functions, formulation of a multi-electron closed-shell electron configuration energy, introduction of core, Coulomb and exchange integrals with their properties, independent particle model, multi-electron atomic Hartree Hamiltonian and related SCF equations solution, vertical ionization potential and Koopman's theorem, Hatree-Fock-Roothaan method for closed cell systems, Roothaan equation, discussion of electron correlation, Condon Slater rule.

Unit-4: Quantum mechanics of molecules

Born-Oppenheimer approximation, Valence bond theory, Molecular orbital treatment for homonuclear molecule, Hückel MO treatment of simple polyenes, separation of electronic and nuclear motion, basis sets for the molecular orbital calculations of polyatomic molecules, configuration interaction calculations of polyatomic molecules, illustrative examples of Ab initio HF and post HF calculations, atomic charge and bonding indices in polyatomic molecules.

Recommended Books

1. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 3rd edition (1997), Oxford University Press. Oxford.
2. I. N. Levine, Quantum Chemistry, 5th edition (2000), Pearson Educ., Inc., New Delhi.
3. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach, (1998), Viva Books, New Delhi.
4. A. K. Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata McGraw Hill, New Delhi.
5. L. Pauling and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, (1935), McGraw Hill, New York.
6. G. C. Schatz and M. A. Ratner, *Quantum Mechanics in Chemistry*, Dover Publication, Inc, New York, 2002.
7. Richard L. Liboff, Introductory Quantum Mechanics
8. D. J. Grffiths, Introduction to Quantum Mechanics
9. J. L. Powell, B. Crasemann, Quantum Mechanics
10. R. K. Prasad, Quantum Mechanics

MCH-306: Advanced Topics in Inorganic Chemistry I

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Redox Reaction

General remark, complementary and non-complementary redox reactions, outer-sphere reaction, inner-sphere reaction, effect of bridging ligand in inner-sphere reaction, kinetics and mechanism, electron tunneling hypothesis, heteronuclear redox reaction and simplified Marcus theory, Marcus cross relationship and its application, remote attack, doubly-bridged process, ligand exchange, intervalence electron transfer, induced reaction, electron transport in biological systems and their simulations

Unit-2: Crystalline solid

Single crystal and poly crystal (twinning problem) lattice, unit cell-primitive and non-primitive unit cells, unit cell parameters and crystal systems. Space group-Hermann–Mauguin notations, space group in triclinic and monoclinic system. Indexing of lattice planes, Miller indices. Bragg's equation, reciprocal lattice and its relation to direct lattice; Bragg's reflection in terms of reciprocal lattice-sphere of reflection and limiting sphere; relation between d_{hkl} and lattice parameters.

Unit-3: Main-group clusters

Geometric and electronic structure, three-, four- and higher connect clusters, the *closo, nido, arachno*-borane structural paradigm**,** Styx No. of neutral and boron hydrides, Wade Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity of the clusters compounds.

Recommended Books

1. F. A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John-Wiley & Sons,New York.
2. James E. Huheey, Inorganic Chemistry, 4th Edn. (1993), Addison Wesley Pub. Co., New York
3. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn. (1997), Butterworth Heinemann, London.

MCH-307: Pericyclic and Photochemistry

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Concept on M.O. and V.B. theory

Introduction to H*ü*ckel molecular orbital (MO) method as a mean to explain modern theoretical methods. Advanced techniques in PMO and FMO theory.Molecular mechanics, semi empirical methods and Ab Initio methods. Pictorial Representation of MOs for molecules, Qualitative Application of MO Theory to reactivity, Valence bond configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams.

Unit-2: Pericyclic reaction

Introduction, phase and symmetry of orbitals, types of pericyclic reactions; Cycloaddition reactions: definition, FMO-approach, co-relation diagram, Dewar's PMO-approach for cycloaddition (2+2 and 4+2) reactions, Woodward-Hoffmann selection rules, regioselectivity, secondary orbital interaction, Lewis acid catalysis, site selectivity, periselectivity. Regioselectivity in 1,3-Dipolar cycloadditions, Electrocyclic reactions: definition, FMO-approach, Dewar's PMO-approach for electrocyclic reactions, electroreversion, stereochemical effects, Woodward-Hoffmann rules, Chelotropic reactions: definition, FMO-approach for cholatropic reactions, Woodward-Hoffmann rules, stereochemical outcome, Sigmatropic rearrangement: definition, types of sigmatropic reactions, Hydrogen shifts and carbon shifts ([1, j] and [i, j]), FMO-approach, Dewar's aromatic transition state approach, selection rules, Claisen and Cope rearrangements, Ene reaction: definition, FMO-approach for ene reactions, effects of Lewis acids.

Unit-3: Organic Photochemistry

Basic Principles, Jablonski diagram, excited state (S1 and T1) of some organic molecules, Cis-trans mechanism, photo chemical reactions of carbonyl compounds, olefins and conjugated carboyl compounds, photo induced functionalisation of organic molecules involving Norrish type I, Norrish type II, Paterno Buchi Reaction, di-π- methane rearrangement, photo reduction of ketones, substitution in aromatic system.

Recommended Books

1. S.M. Mukherjee and S.P. Singh, Pericyclic Reactions &Photochemistry, MacMillan India, New Delhi.
2. I. Fleming, Pericyclic Reactions, Oxford University Press, Oxford (1999).
3.Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2001.
4. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
5. S. M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, Ist Edition (1990), Macmillan India Ltd., New Delhi.
6. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi.

MCH-308: Solid State Chemistry

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Crystal structure and X-ray diffraction

Definitions related to crystal structure, reciprocal lattice, Brillouin Zones, structure factor, Laue equations and Bragg's law, X-ray diffraction experiments: powder method and single crystal method.

Unit-2: Solid State reactions & Phase transitions

General principles and experimental procedure of solid state reactions, growth of single crystals: Czochralski method, Bridgman and Stockbarger methods. Thermodynamic and Burger's classification of phase transition, kinetics of phase transition, nucleation and growth.

Unit-3: Free electron & Band theory of solids

Free electron gas model of metals, free electron gas in a one-dimensional and three dimensional box, Bloch theorem, Kronig-Penny model, tight binding approximation, Band theory of insulators and semiconductors, intrinsic semiconductors, extrinsic semiconductors, doped semiconductors, rectifiers, transistors, p-n junctions and their applications, Schottky and Frenkel defects, stoichimetric imbalance, origin of colours.

Unit-4: Thermal & Magnetic properties of solids

Electronic specific heat, lattice heat capacity, Hall effect, Einstein theory, Debye theory, Born's modification of the Debye theory. Origin and classifications of magnetic substance, magnetic moment, ferromagnetic, antiferromagentic and ferromagnetic ordering, magnetic susceptibility, Curie and Cuire-Weiss law, super exchange, magnetic domains, and hysteresis.

Recommended Books

1. C. Kittel, Introduction to Solid State Physics, John Wiley & Sons, Inc., New York, Chichester.
2. O. Madelung, Introduction to Solid State Theory
3. A. R. West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore.
4. L.V. Azaroff, Introduction to Solids, (1977) Tata McGraw-Hill, New Delhi.
5. A. J. Dekker, Solid State Physics, Prentice Hall

MCH-309: Supramolecular Chemistry & Drug Design

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Supramolecular Chemistry

Fundamentals: definitions of supramolecular chemistry, host-guest chemistry, chelate and macrocyclic effects, preorganisation, thermodynamic and kinetic selectivity, supramolecular interactions (i..e. cation –π, π-π etc.), cation, anion and neutral molecule binding: crown ethers, podands/ lariat ethers, spherands, cryptands, complexation of organic cations, calixarenes, cation host to anion host, shape selectivity, guanidinium receptors, coordination interactions, cavitands: cyclodextrins and molecular tweezers. molecular switches.

Catenanes, rotaxanes and molecular knots: Self assembly and templates, strict self assembly and self assembly with covalent modification, electrostatic and H-bonding effects in templating, catenanes/ catenands/ catenates, rotaxanes/ pseudo-rotaxanes, metal templates for catenanes (Sauvage), π stacking in catenane and rotaxane formation (Stoddart), helicates and molecular knots. *Molecular devices:* history and future of nanoscale machines, relation to host-guest chemistry (definition of supramolecular device), supramolecular photochemistry, photo- and electro-chemical sensors, dendrimers, molecular device components, machines based on catenanes/ rotaxanes, chemically assembled electronic nanocomputing.

Unit-2: Drug design and Antineoplastic agent

Concept of pharmacodynamics, d*rug targets:* enzymes, receptors, nucleic acids; c*oncept on pharmacokinetics:* drug absorption, distribution, metabolism and excretion, concept on lead compound and lead modification, pharmacophore, concept of prodrug and soft drug, structure activity relationship (SAR), factors affecting bioactivity; *Antineoplastic agents*: synthesis and mode of action of mechlorethamine, cyclophosphamide, melphalan, and 6-mercaptopurine. *Cardiovascular drugs:* introduction to cardiovascular diseases, synthesis and mode of action of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyl dopa; *local antiinfective drugs and antibiotics:* synthesis and mode of action of sulphonamides, nalidixic acid, norfloxacin, aminosalicyclic acid, ethinamide, fluconazole, chloroquin and premaquin; *Antibiotics*: cell wall biosynthesis, inhibit-lactam rings, synthesis of penicillin.

Recommended Books

1. J. M. Lehn, Supramolecular Chemistry- Concepts and Perspectives
2. Schneider, H. J., Yatsimirski, Principles and Methods in Supramolecular Chemistry
3. Advanced Organic Chemistry, Part-A, F.A. Carey and R.J. Sundburg
4. Advanced Organic Chemistry, Part-B, F.A. Carey and R.J. Sundburg

MCH-310: Nuclear Chemistry

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Theory of radioactive decay

Quantum mechanical aspects of radioactive disintegration, alpha decay paradox and its explanation in terms of tunnel effect, Geiger-Muller relationship, time-dependant perturbation theory, Golden rule and its application in explaining beta and gamma transition, selection rules.

Unit-2: Nuclear force and structures

Two body problem - properties of deuteron and derivation of depth-range relationship, its applications in explaining nature of nuclear force, elementary particles; nuclear models - strong and weak interaction, nuclear magnetic dipole moment and electric quadruple moment in terms of shell model, collective model, Fermi gas model.

Unit-3: Nuclear reactions general features

Types of nuclear reaction, conservation laws, nuclear reaction dynamics, mechanism of nuclear reaction, use of uncertainty principle, resonance and non-resonance reaction, optical model and calculation of mean free path, nuclear fission and fusion reaction, calculation of fission probability from Bohr-Wheeler's theory Centre of mass system and laboratory co-ordinate.

Unit-4: Nuclear detectors

Classification of nuclear detectors, G. M. detector-operational principle, dead time, proportional detectors: proportional counter performance, flow-type proportional counter, gas multiplication factor, scintillation detectors: different types with examples, pulse shape analysis, resolution and detection efficiency, liquid scintillation detectors, detection of neutrons, semiconductor detector: general characterization, depletion depth, reverse bias, requirement of cryogenic condition, resolution and efficiency, pulse rise time, with a brief account of n-type and p-type semiconductor, Si lattice, Ge-Li, Si-Li - a comparison intrinsic and doped-semiconductor-fabrication surface barrier detector; some basic ideas of pulse processing and shaping, single- and multi-channel analysers, digital and analogue systems, applications in space research, development of detector assembly with requirement of newer space and defence technology viz., nuclear missile, Coincidence counting Determination of absolute disintegration rates, decay scheme studies.

Recommended Books

1. B. Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, New York, 1965.
2. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th Edn Reprint, New Age International (P) Ltd Publications, New Delhi, 2001.
3. G. R. Choppin and J. Rydberg, Nuclear Chemistry: Theory and Applications, Pergamon, Oxford, 1980.
4. D. D. Sood, A.V. R Reddy and N. Ramamoorty, Fundumentals of Radiochemistry, Yancas, Mumbai, 2004.

MCH-391: Inorganic Chemistry Lab III

L-T-P: 0-0-9 **Credit: 6**

- To study the kinetics of different inorganic reactions by conductometric, colorimetric, and spectrophotometric method
- Estimation of selected ores, minerals, and alloys
- Synthesis and characterization of different coordination complexes

MCH-392: Organic Chemistry Lab III

L-T-P: 0-0-9 **Credit: 6**

- Qualitative analysis of liquid sample (color, odour, solubility etc.); *Thin Layer Chromatography (TLC, preparation of TLC plates, analysis),* boiling point determination; functional groups tests, UV-VIS spectral characterizations: (measure λ_{max}, and explain), *Assign* ^{1}*H-NMR,* ^{13}*C-NMR spectra,* Identify the liquid substance.
- *Extraction of Renewable chemicals:* Take a particular part of a plant such as fruit, leaf, bark, heavy wood, etc. Weight it. Extract with a particular solvent. Remove the volatiles. Purify. Weigh the product. Calculate % yield, Analyze the product by Thin Layer Chromatography, calculate R_f value. UV-VIS spectral characterizations: measure λ_{max},and explain. Submit the product with proper label.
- *Quantitative Estimation of:* (a) Sugars (Glucose, Cane sugar), (b) Phenol, (c) Aniline, (d) Nitrogen by Kjldahl method, (e) Saponification and Iodine value.

MCH-393: Physical Chemistry Lab III

L-T-P: 0-0-9 **Credit: 6**

- Synthesis, characterization and applications of nanomaterials
- Synthesis and characterization of polymers utilizing different polymerization techniques

Recommended Books

1. A.I. Vogel, Qualitative Inorganic Analysis
2. A.I. Vogel, A Textbook of Quantitative Inorganic Analysis, ELBS
3. Ghosal, Mahaparta and Nad, An Advanced Course in Practical chemistry
4. G. N. Mukherjee, Handbook of Practical Chemistry
5. A.I. Vogel, A Textbook of Practical Organic Chemistry
6. A. M. James, F. F. Prichard, Practical Physical Chemistry
7. Shoermaker, Garland, Experimental Physical Chemistry

Detailed Syllabus of Fourth semester

MCH-401: Spectroscopy for Structure Elucidation

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Ultra-Violet & Infrared spectroscopy

Absorption of dienes, polyenes, carbonyl compounds and α,β-unsaturated carbonyl compounds, Woodward rule and its applications. Different vibration modes, bond stretching, absorption region of functional groups, electrical and steric effects, effects of hydrogen bonding, Fingerprint region and interpretation of IR spectra.

Unit-2: NMR spectroscopy

Principles, relaxation phenomenon, chemical shifts, coupling constants, spin-spin interactions, simplification of complex spectrum, spin decoupling, nuclear Overhauser effect, detailed interpretation of ^{1}H NMR, ^{13}C NMR, DEPT, two dimensional NMR: COSY, NOESY.

NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, ^{11}B, ^{19}F, ^{27}Al, and ^{31}P – NMR spectroscopy with typical examples.

Unit-3: Mass spectroscopy

Principles, different techniques, fragmentation modes, factors influencing ion abundance, rearrangements, cleavage associated with common functional groups, molecular and metastable ion peak, Nitrogen rule and interpretation of mass spectra.

Combined applications of different spectroscopic techniques (UV, IR, NMR, Mass) in elucidation of structure.

Unit-4: EPR & Mössbauer

Origin, principle, hyperfine splitting, factors affecting the magnitude of g-value, anisotropy in hyperfine coupling constants, zero-field splitting, Kramers' degeneracy, nuclear quadrupole interactions, Mössbauer effect, isomer shift, quadrupole splitting, typical spectra of iron and tin compounds, NQR.

Unit-5: Optical rotatory dispersion & Circular dichroism

Principles of ORD and CD, different techniques, Cotton effect, Faraday and Kerr effects, applications in determining absolute configuration of metal complexes, amino acids and proteins.

Recommended Books

1. R. M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, 6th Edition (2003) John Wiley, New York.
2. D. H. Williams and I.F. Fleming, Spectroscopic Methods in Organic Chemistry, 4th Edition (1988), Tata-McGraw Hill, New Delhi.
3. P. Y Bruice, Organic Chemistry, 2nd Edition (1998) Prentice-Hall, New Delhi.
4. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edition (1987), Blackwell Scientific Publications, Oxford, London.
5. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.
6. R. S. Drago, Physical Methods in Inorganic Chemistry, 1st Edition (1971), Affiliated East-West Press, New Delhi.

MCH-402: Polymer and Materials Chemistry

L-T-P: 3-1-0 **Credit: 4**

Unit-1: Polymer Chemistry

Introduction, classification, different molecular weights and their determination, polymerization techniques, detailed kinetics of condensation and addition polymerization, controlled polymerizations, sequence and stereo-controlled polymer synthesis, properties of polymers in solutions, Flory-Huggins model, glass transition temperature, crystallinity, mechanical properties, polymer modification and manufacturing of commodity polymers: grafting, cross-linking, blending, compounding.

Specialty polymers: Liquid crystalline polymers, conducting polymers, electroluminescent polymers, inorganic polymer, biomedical polymers, and hybrid materials based on polymers.

Unit-2: Material Chemistry

Introduction, importance, classifications and theoretical aspect of nanomaterials, top down-bottom up approach, different synthetic strategy of metal/metal oxide/semiconducting materials, template based synthesis, size, shape and dimension controlled synthesis, growth kinetics, composite nanostructures, properties and size effect of nanomaterials: optoelectronic, mechanical, magnetic, and catalytic properties, applications of nanomaterials.

Different Instrumental Techniques for characterization: Basic principles and applications of X-ray diffraction, electron microscopies (SEM, TEM), scanning probe microscopies (STM), atomic force microscopy (AFM), optical microscopies [confocal microscopy, scanning near field optical microscopy, particle size analysis (DLS)], thermal (DSC, DTA), optical (IR, FTIR, Raman) and XPS.

Recommended Books

1. G. Odian, Principles of Polymerization, 3rd Edition (1991), John Wiley, Singapore
2. F. W. Billmayer, Jr., Text Book of Polymer Science, 3rd Edition (1984), Willey-Interscience, NY
3. C. Tanford, Physical Chemistry of Macromolecules
4. P. Bahadur, N.V. Sastry, Principle of Polymer Sciences, Narosa Publishing House, New Delhi
5. V.R. Gowarikar, N.V. Vishwanathan, J. Shreedhar, Polymer Sciences, Wiley Eastern, New Delhi
6. P. W. Atkins, Physical Chemistry, 8th Edition, Oxford University Press, New York
7. P. J. Flory, Polymer Chemistry
8. C. N. R. Rao, A. Müller, A. K. Cheetham, The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Vols 1 and 2, Wiley-VCH, Weinheim, 2004
9. C. Bréchignac, P. Houdy, M. Lahmani, Nanomaterials and Nanochemistry, Springer, London, 2006.
10. G. Cao, Nanostructures & Nanomaterials, Synthesis, Properties & Applications, Imperial College Press, London, 2004. L. Cademartiri and G. A. Ozin, Concepts of Nanochemistry, Wiley-VCH, Weinheim, 2009.
11. C. N. R. Rao, A. Muller and A. K. Cheetham, Nanomaterials Chemistry: Recent Developments and New Directions, Wiley-VCH, Weinheim, Germany, 2007.
12. G.A. Ozin, A. C. Arsenault and L. Cadematiri, Nanochemistry: A Chemical approach to Nanomaterials, Royal Society of Chemistry, London, 2009.

MCH-403: Inorganic Reaction Mechanism & Photochemistry

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Inorganic reaction mechanism

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, reactions without metal-ligand bond breaking, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters-tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand; reactions in fluxional organometallic compounds.

Unit-2: Photochemistry of Transition metal complexes

Photoreactions of complexes of Cr(III) and Co(III), photo-aquation, photo-substitution and photo-racemization, photochemistry of $Ru(bpy)_3^{2+}$ and its application as photocatalyst for photo-splitting of water, photooxidation of 2-propanol and photo-reduction of carbon dioxide, cyanide bridged triruthenium(II) bipy complexes as antenna, photochemistry of diisocyanide bridged diimers of Rh(I), applications of quenching and sensitization techniques in the identification of reactive state in coordination complexes, photochemistry of transition metal carbonyls and europium complexes.

Recommended Books

1. J. O. Edwards and W. A. Benjamin, Inorganic Reactions Mechanism, INC, New York, 1965.
2. C. H. Langford and H. B. Gray, Ligand Substitution Processes, W. A. Benjamin, New York, 1966.
3. F. Basolo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Edn, Wiley, New York, 1967.
4. D. Katakis and G. Gordon, Mechanisms of Inorganic Reactions, John Wiley & Sons, New York, 1987.
5. R. G. Wilkinns, Kinetics and Mechanism of Reactions of Transition Metal Complexes, 2nd Edn, VCH, Weinheim, 1991.
6. D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, New York and London (1994).
7. G. J. Ferraudi, Elements of Inorganic Photochemistry, John Wiley & Sons (1988).
8. V. Balzani and V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, London (1970).
9. O. Horvath and K.L. Stevenson, Charge Transfer Photochemistry of Coordination Complexes, VCH Publishers Inc. (1993)

MCH-404: Advanced Organic Synthesis II

L-T-P: 3-0-0 **Credit: 3**

Unit-1: The Disconnection approach

Basic principles, guidelines for disconnection with special emphasis on chemoselective, regioselective, stereoselective and stereospecific reactions, functional group inter conversion, synthon and reagent, synthetic equivalent, illogical electrophile and illogical nucleophile, Umpolong synthesis. designing synthesis of some target molecules with proper retrosynthetic analysis : Menthol, Taxol, Penicillin V, Reserpine, Progesterone, Estrone, Periplanone B, L-Hexoses etc.

Unit-2: Special techniques in Organic synthesis

The background of organic synthesis, reactions with solid-supported reagents and catalyst, solid phase synthesis, Phase transfer reactions, Sonochemistry, Microwave in organic synthesis, Ionic liquid in organic synthesis, Electro organic synthesis, Concept of organocatalyst.

Unit-3: Asymmetric synthesis

Introduction, kinetic and thermodynamic principles to asymmetric synthesis, diastereoselective & enantioselective synthesis; *Methods of asymmetric synthesis:* Resolution, use of chiral pool, chiral auxiliaries, use of stoichiometric chiral reagents, asymmetric catalysis. Asymmetric hydrogenation with special reference to Ru-BINAP catalysts, asymmetric reduction of prochiral ketones with Baker's Yeast & CBS-catalyst, asymmetric epoxidation with special reference to Sharpless and Jacobsen epoxidation, asymmetric diethylzinc addition to carbonyl compounds, asymmetric aldol reactions, asymmetric Michael reaction; industrial applications of asymmetric synthesis.

Unit-4: Organometallic chemistry

Preparation, properties and reactions of Organomagnesium, Organolithium and Organozinc reagents in synthesis. The role of Boron, Silicon, Sulphur and Phosphorus in organic synthesis. Principle, preparation, properties and application of some transition metals in organic synthesis with special reference to Copper, Palladium, Cobalt, Titanium and Nickel.

Unit-5: Green chemistry

The need of green chemistry, Principles of green chemistry, Concept of atom economy Tools of green Chemistry – microwave, ultra sound, ionic liquids, supercritical H_2O and CO_2 as solvents, etc. Green Chemistry in real world cases and planning green synthesis in chemical laboratory.

Recommended Books

1. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2001.
2. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
3. R. O. C. Norman and J. M. Coxon, Principle of organic synthesis
4. S. Warren, Organic synthesis: The disconnection approach
5. W. Carruthers, Modern methods of organic synthesis
6. Paul. T. Anantas and Tracy C. Williamson, Green Chemistry
7. Theory and Practice, Paul T. Anastas and John C. Warner, Green Chemistry

MCH-405: Electrochemistry

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Ion-Solvent interaction

Born model and Born equation, enthalpy of ion-solvent interaction and its evaluation, Eley-Evan model, solvation number and its determination

Unit-2: Electrical double Layer

OHP and IHP, potential profile across double layer region, potential difference across electrified interface, structure of the double layer**:** Helmholtz-Perrin, Gouy-Chapman, and Stern models, Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot, thermodynamics of double layer, electrocapillary equation, determination of surface excess and other electrical parameters.

Unit-3: Electrode Kinetics

Polarizable and non-polarizable interfaces, multistep reactions: a near equilibrium relation between current density and over potential, concept of rate determining step, determination of reaction order, stochiometric number, transfer coefficient.

Unit-4: Applications

Electrochemical cell, fuel cell, electrocatalysis, corrosion, and cyclic voltammetry etc.

Recommended Books

1. J. O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 1 & 2A and 2B, (1998) Plenum Press, New York.
2. A. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd edition, (2001) John Wiley &Sons, New York.
3. Samuel Glasstone, An Introduction to Electrochemistry: Edition 1st, East-West Press Pvt Ltd New Delhi, India.
4. S. R. Morrison, Electrochemistry in Semiconductor and Oxidised Metal Electrodes, Plenum Press, New York, 1980.
5. D. E. Kyriacou and D. A. Jannakoudis, Electrocatalysis for Organic Synthesis, Wiley, New York, 1986.
6. J. Goodisman, Electrochemistry: Theoretical Foundations, Wiley, New York, 1987.
7. J. O'M. Bockris and S. U. M. Khan, Surface Electrochemistry, Plenum Press, New York, 1993.
8. C. M. A. Brett and A. M. O. Brett, Electrochemistry: Principles, Methods and Applications, Oxford University Press, Oxford, 1993.
9. P. W. Atkins, Physical Chemistry, 5th Edn, Oxford University Press, Oxford, 1994.
10. K. V. Kordesch, Fuel Cells and Their Applications, VCH, Weinheim, 1994.

MCH-406: Advanced Topics in Inorganic Chemistry II

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Magnetochemistry

Types of magnetic materials, magnetic susceptibility and its determination: Gouy, Faraday and Evans methods, vibrating sample magnetometer, SQUID and NMR methods. Magnetic anisotropy, diamagnetism in atoms and polyatomic systems, Pascal's constants, Lande interval rule, energies of J states, Curie equation, Curies law and Curie-Weiss law, First order and second order Zeeman effects, temperature independent para magnetism, simplification and application of Van Vleck susceptibility equation, quenching of magnetic moments of transition metal compounds in cubic and axially symmetric crystal fields, low spin- high spin crosser, magnetic behaviour of Lanthanides and Actinides, magnetic exchange interactions, magnetic materials.

Unit-2: Cluster, Cage, Ring of main group transition-metal clusters

Capping rules, metal-ligand complexes vs heteronuclear cluster, isolobal analogs of p-block and d-block clusters, limitations and exceptions, clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters, metal-carbonyl clusters, structures, capping and electron counting, molecular clusters in catalysis, clusters to materials, boron-carbides and metalborides, illustrative examples from recent literature.

Unit-3: Inorganic Polymers

Classification, types of inorganic polymerization, comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulphur-nitrogen, sulphur-nitrogen-fluorine compounds, binary and multi-component systems, hemolytic inorganic systems.

Recommended Books

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John-Wiley & Sons, New York.
2. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn. (1997), Butterworth Heinemann, London.
3. F. E. Mabbs and D. J. Machin, Magnetism and Transition Metal Complexes, Dover Publications, New York, 2008.
4.O. Kahn, Molecular Magnetism, VCH, New York, 1993.
5. P. Day and A. E. Underhill (Eds), Metal-organic and Organic Molecular Magnets, RSC, London, 2000.
6. J. S. Miller and M. Drillon (Eds), Magnetism: Molecules to Materials, V; Molecule-based Magnets, Wiley-VCH, Weinheim, 2005.
7. B. D. Cullity and C. D. Graham, Introduction to Magnetic Materials, 2nd Ed, John Wiley & Sons, New York, 2011.
8. F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, Chichester, 1991.20 20
9. V. Balzani and F. Scandola, Supramolecular Photochemistry, Ellis Horwood, Chichester, 1991.
10. J. -M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim, 1995.
11. J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 2nd Ed, John Wiley & Sons.

MCH-407: Heterocyclic Chemistry

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Fundamentals

Nomenclature of heterocycles: replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles; *aromatic heterocycles:* tautomerism in heterocyclic systems, reactivity of aromatic heterocycles; *non-aromatic heterocycles:* conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction, anomeric and related effects, hydrogen bonding and intermolecular nucleophilic-electrophilic interactions; *meso-ionic systems:* general classification, chemistry of some important meso-ionic heterocycles of type A and B and their applications.

Unit-2: Heterocyclic synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions; synthesis and reactivity of 3-, 4-, 5- 6- & 7-membered heterocycles with one, two or more heteroatoms (aziridines, oxiranes, thiiranes, azetidines, oxetanes, thietanes, diazines, triazines, thiazines, azepines, oxepines); *benzo-fused five and six-membered heterocycles:* synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, benzothiophenes, quinolizinium and benzopyrylium salts, coumarins and chromones; heterocycles in pharmaceutical industry.

Recommended Books

1. J. A. Joule and K. Mills: Heterocyclic Chemistry (4 th Edition)
2. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press, 2001.
3. M.B. Smith & Jerry March, March's Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
4. Advanced Organic Chemistry, Part-A, F.A. Carey and R.J. Sundburg
5. Advanced Organic Chemistry, Part-B, F.A. Carey and R.J. Sundburg

MCH-408: Statistical Mechanics

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Ensembles and Partition function

Probability, Equal a priori probability, concept of ensemble, Micro/Macro/Grand-canonical ensemble, Ergodic hypothesis, phase space, quantization of phase space, Liouville theorem, review of rotational, vibrational and translational partition functions, entropy of a two level system, Gibbs paradox, equipartition of energy, applications of partition function to specific heat of solids, chemical equilibrium ideal and real gases.

Unit-2: Quantum statistics

Bose-Einstein distribution law, Einstein condensation, thermodynamic properties of ideal BE gas, Fermi-Dirac distribution law, degenerate Fermi gas, electron in metals, magnetic susceptibility.

Unit-3: Fluctuations

Mean square deviation and fluctuation in ensembles, concentration fluctuation in quantum statistics.

Unit-4: Non-equilibrium states, irreversible thermodynamics

Conservation of mass and energy in open systems, entropy production in chemical reactions, entropy flow in open systems, forces and fluxes, linear phenomenological laws, Onsager's reciprocity or reciprocal relation, validity of Onsager equation and its verification, principle of microscopic reversibility, stationary non-equilibrium states, Curie-Prigogine principle and its applications.

Boltzmann transport equation, particle diffusion, and electrical conductivity.

Recommended Books

1. B. K. Agarwal and M. Eisner, Statistical Mechanics, (1988) Wiley Eastern, New Delhi
2. D. A. McQuarrie, Statistical mechanics, (1976) Harper and Row Publishers, New York
3. E. S. R. Gopal, Statistical Mechanics and Properties of Matter, Ellis Horwood, England, 1974
4. S. K. Ma, Statistical Mechanics, World Sci, Singapore, 1985
5. R. K. Pathria, Statistical Mechanics, Butterworth-Heinemann, 1996
6. B.B. Laud, Statistical Mechanics

MCH-409: Chemical Applications of Group Theory

L-T-P: 3-0-0 **Credit: 3**

Unit-1: IR and Raman spectroscopy

Brief introduction to molecular vibrations, selection rules for fundamental transitions, symmetry of normal modes of molecules, Infrared and Raman activity of some typical molecules (molecules of C_{2v}, C_{3v}, C_{4v}, D_{2h}, D_{3h}, D_{4h}, Td and Oh point groups).

Unit-2: Molecular Orbital theory

Introduction, transformation properties of atomic orbitals, hybridization schemes for σ and π bonding, hybrid orbitals as LCAOs, construction of SALC's and their use in calculation of π MO's under the H*ü*ckel approximations, calculation of MO's of AB_n type and sandwitch type molecules, study of hybridization, selection rules, allowedness/forbiddenness of n-π^* and π-π^* transitions, splitting of terms in octahedral and tetrahedral ligand fields, Orgel and Tanabe-Sugano diagrams.

Recommended Books

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn. (1999), John Wiley & Sons, New York.
2. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 2nd Edn. (1999), Prentice Hall International Inc., London.
3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International Pvt. Ltd., New Delhi (1999).
4. A. Vincent, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
5. D. M. Bishop, Group Theory and Chemistry, Oxford University Press, 1993.
6. V. Heine, Group Theory in Quantum Mechanics: An Introduction to Its Present Usage, Dover Publication, New York, 1991.
7. R. McWeeny, Symmetry: An Introduction to Group Theory and Its Applications, Dover Publications, New York.

MCH-410: Advanced Spectroscopy

L-T-P: 3-0-0 **Credit: 3**

Unit-1: Fundamentals

Generation of singlet and triplet states, radiative and non-radiative transitions, fluorescence, phosphorescence, quantum yield and life-time measurements, fluorescence quenching, resonance energy transfer, solvation dynamics.

Unit-2: Laser Spectroscopy

Brief review of laser action, application of lasers as excitation source, time resolved fluorimetry, transient absorption spectroscopy, surface plasmon spectroscopy, multiphoton spectroscopy, single molecule spectroscopy, fluorescence correlation spectroscopy, upconversion, microscopy (optical, phase contrast, confocal, FLIM), SERS, and CARS.

Unit-3: Photophysical Processes

Unimolecular processes, delayed fluorescence, kinetics of bimolecular processes: collision quenching, Stern-Volmer equation, concentration dependence of quenching and excimer formation, excited state electron transfer processes: exciplex, twisted intramolecular charge transfer processes, proton couple electron transfer processes, special photochemical reactions, flash photolysis, laser flash photolysis.

Recommended Books

1. J. M. Hollas, Modern Spectroscopy, Wiley, New York, 1996.
2. D. N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, University Press, 2001.
3. G. Aruldhas, Molecular Structure and Spectroscopy, 2nd Edn, Prentice-Hall of India, New Delhi, 2007.
4. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill International Book Company, Tokyo, 1982.
5. J. D. Graybeal, Molecular Spectroscopy, McGraw-Hill International Editions, Spectroscopy series, 1998.
6. J. R. Lakowicz, Principles of Fluorescence Spectroscopy
7. R. Schinke, Photodissociation dynamics
8. W. Demtroder, Laser spectroscopy
9. R. D. Levine, Molecular Reaction Dynamics
10. J. I. Steinfeld, J. S. Francisco, W. L. Hase, Chemical Kinetics and Dynamics