



UNIVERSITY OF CALCUTTA

Notification No. CSR/ 68 /18

It is notified for information of all concerned that the Syndicate in its meeting held on 13.07.2018 (vide Item No.11) approved the Syllabus of Two-Year (Four-Semester) M.Sc. Course of Study in Chemistry under CBCS in the Post-Graduate Departments of the University and in the affiliated Colleges offering Post-Graduate Courses under this University, as laid down in the accompanying pamphlet.

The above shall be effective from the academic session 2018-2019.

SENATE HOUSE
KOLKATA-700073
The 17th August, 2018


(Debabrata Manna)

Deputy Registrar (Acting)

SYLLABUS

FOR

TWO-YEAR FOUR-SEMESTER COURSE IN

CHEMISTRY

2018

UNIVERSITY OF CALCUTTA

DEPARTMENT OF CHEMISTRY

UNIVERSITY OF CALCUTTA

TWO YEAR FOUR-SEMESTER M.Sc. COURSE IN CHEMISTRY

COURSE STRUCTURE

DURATION	SEMESTER				TOTAL MARKS
	I JULY-DEC	II JAN-JULY	III JULY-DEC	IV JAN-JUNE	
MARKS	250	250	250	250	1000
COURSE TYPE	THEO PRACT	THEO PRACT	THEO PRACT	THEO PRACT	
GENERAL (G)	150 100	150 100	50		650
CREDIT POINTS	(12) (8)	(12) (8)	(4)		(52)
CBCS			100		
CREDIT POINTS			(8)		

SPECIAL (S)			100	150 100	350
CREDIT POINTS			(8)	(12) (8)	(28)
Total Marks	150 100	150 100	150 100	150 100	1000 (80)

Total credit points: **80**

Special Courses (S) in Four Branches of Chemistry are

- (i) Analytical Special (SA)
- (ii) Inorganic Special (SI)
- (iii) Organic Special (SO)
- (iv) Physical Special (SP)

SEMESTER – I (Marks – 250)

Course ID	Marks/Credit			
	Theo	Credit	Pract	Credit
CHEM – G11	50	4	-	-
CHEM – G12	50	4	-	-
CHEM – G13	50	4	-	-
CHEM – G14	-	-	100	8
Total	150	12	100	8

SEMESTER –II (Marks – 250)

Course ID	Marks/Credit			
	Theo	Credit	Practical	Credit
CHEM – G21	50	4	-	-
CHEM – G22	50	4	-	-
CHEM – G23	50	4	-	-
CHEM – G24	-	-	100	8
Total	150	12	100	8

SEMESTER –III (Marks – 250)

Course ID	Marks/Credit			
	Theo	Credit	Practical	Credit
CHEM – G31	50	4	-	-
CBCC-A	50	4	-	-

CBCC-B	50	4	-	-
CHEM–SA31/SI31/SO31/SP31	-	-	100	8
Total	150	12	100	8

SEMESTER –IV (Marks – 250)

Course ID	Marks/Credit			
	Theo	Credit	Practical	Credit
**CHEM – SA41/SI41/SO41/SP41	50	4	-	-
**CHEM – SA42/SI42/SO42/SP42	50	4	-	-
**CHEM – SA43/SI43/SO43/SP43	50	4	-	-
*CHEM – SA44/SI44/SO44/SP44	-	-	100	8
Total	150	12	100	8

* Review and project work

** One special course to be opted and continued systematically

Course Structure and marks distribution

1. Theoretical papers

Full marks: 50, each paper

Each unit 10 marks, two questions per unit to be set and any one to be answered

2. Practical Papers

Full Marks: 100, each paper

Course ID	Experiment	General Laboratory performance	*Seminar
CHEM-G14	45	45	10
CHEM-G24	45	45	10
CHEM – SA31/SI31/SO31/SP31	50	50	-

- Topic should be outside the UG curriculum of CU; use of overhead/LCD projector is mandatory ; time 10m, followed by discussion

Course ID	*Continuous assessment	Review	Project	Grand Viva
CHEM – SA44/SI44/SO441/SP44	10	25	40	25

*Continuous assessment to be assessed by the guide

Review (maximum 3000 words excluding references and figures) and Project to be assessed by External Expert

Grand Viva to be taken by Sectional Faculty members and assessed by them

SYLLABUS

SEMESTER – I

Course ID: CHEM-G11

Unit-1: Symmetry

Symmetry elements; Symmetry operations; Group theory; Group multiplication table;

Point group; Schönflies symbols; Classes of point groups; Platonic solids; Stereographic

Projections

Unit-2: Coordination Chemistry

Crystal field theory, Splitting of d orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal, octahedral and pentagonal bipyramidal fields of similar and dissimilar ligands. Crystal field stabilization energies in weak field and strong field environments, octahedral site preference energy, tetragonal distortion and Jahn Teller effect. Shapes of complexes. Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stability of complexes (Irving Williams order). Kinetic aspects of crystal field stabilization, crystal field activation energy, labile and inert complexes.

Electronic spectra of transition metal complexes – determination of free ion terms of d^1 to d^9 , microstates, determination of ground and all excited state terms of d^n terms in octahedral and tetrahedral fields, Orgel diagrams (qualitative approach), hole formalism, inversion and equivalence relations, selection rules for spectral transitions, d-d spectra and crystal field parameters, Nephelauxetic series, qualitative idea of Tanabe–Sugano diagrams, charge transfer spectra. Magnetic properties – elementary idea.

Unit-3: EPR and Mössbauer Spectroscopy

Principle of EPR and spin Hamiltonian (comparison to NMR spectroscopy), spectrometer, external standard, line-width, nuclear hyperfine interactions, anisotropy in Lande g factor and hyperfine interaction, magnetically equivalent and non-equivalent set of nuclei, intensity, structural information of organic radical and inorganic molecules from EPR spectra. Mössbauer activity:

principle, experiment, line-width, center shift, quadruple interaction, magnetic interaction; information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in variety of environments.

Unit-4: Bioinorganic Chemistry – 1

Elements of life: basic reactions in biological systems and roles of metal ions. Bioenergetic principle and role of ATP. Metal ion transport and storage proteins: ferritin, transferrin, celluloplasmin. Transport across biological membrane: Na⁺ - K⁺ - ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxypeptidase, urease. Metal dependent diseases: Wilson's disease, Alzheimer disease, Metal complexes as drugs: Pt, Rh, Ru and Au drugs. Toxic effects of metal ions, detoxification by chelation therapy. Cobalamins including vitamin and coenzyme B12. Protective metalloenzymes such as cytochrome P-450, superoxide dismutase, catecholase, peroxidase. Photosynthesis, Chlorophyll, PS-I, PS-II, photosynthetic electron transport chain.

Unit-5: Electrochemical Analysis

Voltammetry: cyclic voltammetry, polarography, anodic stripping voltammetry; Amperometry; Coulometry; Electrogravimetry

Course ID: CHEM-G12

Unit-1: Structure-Activity Relationship

MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes (C₆₀), alternate and non-alternate hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods-Frost diagram. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Hammett equation and its modifications.

Unit-2: Stereochemistry I

Winstein-Holness equation, Curtin-Hammett principle; Conformational analysis of cyclohexane, cyclohexene, decalin and their derivatives; perhydroanthracene, perhydrophenanthrene etc., Felkin-Anh, Cieplak and Zimmerman-Traxler Models; Addition Reactions to Carbonyl Compounds.

Unit-3: Pericyclic Reactions

Introduction to pericyclic reactions, understanding of molecular orbitals of acyclic conjugated systems. Thermal and photochemical pericyclic reactions: electrocyclic reactions, cycloaddition reactions and sigmatropic rearrangements. Rationalization based on Frontier M.O. approach, correlation diagrams, Dewar-Zimmermann approach (concept of aromaticity in the transition states). The Woodward-Hoffmann selection rules. General perturbation molecular orbital theory in cycloaddition reactions; reactivity, regioselectivity and periselectivity in cycloaddition reactions. Sommelet-Hauser, Cope and Claisen rearrangements, Ene reaction, Wittig rearrangement.

Unit-4: NMR Spectroscopy I

Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, classification of A_4 , A_3 , ABX, AMX, ABC, A_2B_2 in proton NMR. Introduction to ^{13}C -NMR spectroscopy, application of NMR spectroscopy and other spectroscopical techniques to simple structural and mechanistic problems. Rules for carbon13 calculations, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation processes, problems on NOE, nuclei with negative NOE.

Unit-5: Natural Products

Familiarity with methods of structure elucidation (chemical & spectroscopical method), biosynthesis, synthesis and biological activity of alkaloids (nicotine, atropine, coniine and papaverine).

Unit-1: Interfacial Chemistry

Curved surfaces: Young-Laplace and Kelvin equations. Adsorption of solids: BET equation. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; micro- and macro-emulsions.

Unit – 2: Atomic Structure

Zeeman effect, fine structure, spin-orbit interaction, effect of high magnetic field, Lande g factor, Atomic (and molecular) terms

Unit-3: Quantum Mechanics 1

Postulates and their analysis. Properties of operators and commutators. Equation of motion. Stationary states, Quantization Schemes, Ehrenfest's theorems, Some properties of one-dimensional systems, Barrier problems and tunneling.

Unit-4: Kinetics 1

Fast reactions, Oscillatory reactions, Autocatalysis. Electrode kinetics: Nernst, Butler-Volmer and Tafel equations.

Unit-5: Polymer Chemistry

Classification of polymers, Kinetics of polymerization, Molecular weight of polymer and its determination, Some specific methods for molecular weight determination of biopolymers- gel filtration, SDS-PAGE for proteins, Agarose gel method for nucleic acids. Thermodynamics of polymer solution: Polymer conformation.

Course ID: CHEM-G14

Practical Chemistry 1

Spectrophotometric, ion exchange and complexometric estimations.

Identification of single organic liquid with one or more functional groups.

Experiments (Kinetics, equilibrium, electrochemistry, spectroscopy)

SEMESTER – II

Course ID: CHEM-G21

Unit-1: Chemical Bonding

Different types of bondings including weak interactions; Valence bond and molecular orbital theories – comparative account; Group orbitals in molecular orbital approach; Molecular orbital description of varieties of dinuclear, trinuclear and oligonuclear molecules, radicals and ions, including metal complexes having geometries such as tetrahedral (T_d), square planar (D_{4h}), octahedral (O_h), etc; Walsh diagram; Evidence of MO pictures from spectra and reactivity; Explanation of spectrochemical and Nephelauxetic series; Molecular term symbols.

Unit-2: Complex Equilibria

Stability of mononuclear, polynuclear mixed ligand complexes in solution, statistical and non statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes, determination of stability constants and composition of complexes by potentiometric, spectrophotometric and polarographic methods, conditional stability constant and application of complexometric titration in analytical chemistry. Solubility equilibria: Quantitativeness of precipitation (of metal hydroxides, sulphides, and chelate complexes).

Unit-3: Organometallic Chemistry – 1

Applications of 18-electron and 16-electron rules to transition metal organometallic complexes. Isolobal and isoelectronic relationships with examples. Structure and bonding in metal-alkyl,-alkene,-alkyne, -allyl (η^1 & η^3), -carbonyl, -carbide and cyclopentadienyl complexes with typical examples. Structure and bonding of $[(PPh_3)_2Pt(C_2Ph_2)]$, $[Mo(\text{porphyrin})(C_2H_2)]$, $[Co_2(CO)_6(C_2Ph_2)]$, $[Ni(\eta^3-C_3H_5)_2]$ and $[FeCp_2]$. Reactions of organometallic complexes: Substitution, oxidative addition,

reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Unit-4: Selected topics on the chemistry of s and p block elements

Structure and bonding in higher boranes based on Lipscomb's topological concept, Wade's rules, borohydride B_nH_{n-2} anion, carboranes, metalloboranes, hydroboration reactions. Alkali metal complexes with macrocyclic ligands (crown ethers, cryptates and spherand). Aqueous and complex chemistry of beryllium and aluminium. Main group organometallic chemistry: classification, synthesis, reaction, structure and bonding, and application of typical examples.

Unit-5: Nuclear chemistry

Nuclear reactions. Nuclear activation analyses. Charged particle activation analyses. Radiotracer methods: study of chemical reactions, nuclear medicine, isotope dilution analysis. Radioanalytical techniques: particle induced X-ray emissions, Rutherford back scattering spectrometry, hot-atom

Course ID: CHEM-G22

Unit-1: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, *Cis-trans* isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane rearrangement, photochemistry of arenes, Photoreaction in solid state. Method of generation and detection (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications; cyclisation of radicals.

Unit-2: Synthetic Methodology I

Organoboron - Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates.

Organophosphorus - Chemistry of organophosphorus compounds, Phosphorus ylides and chiral phosphines.

Unit-3: Synthetic Methodology II

Chemistry of organosilicon compounds, Synthetic uses of silyl ethers, silylenol ethers, TMSiCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer Villiger rearrangement

Unit-4: Synthetic Methodology III

Organosulphur- Chemistry of organosulphur compounds, Sulphur- stabilized anions and cations, sulphonium salts, sulphonium and sulfoxonium ylides, chiral sulfoxides, umpolung

Nitrogen ylide, oxonium ylide

Unit-5: Heterocyclic Chemistry I

Synthesis and reactivity of pyridine, quinoline, isoquinoline, indole, pyrazole, imidazole, oxazole, thiazole, isooxazole and their applications in organic synthesis.

COURSE ID: CHEM-G23

Unit-1: Valency

Approximations in Quantum Chemistry. Born-Oppenheimer (B.O.) approximation. Avoided crossings and beyond B.O. approximation. Virial theorem and chemical bonding. Theories of valence: VB and MO. π -electron Hamiltonians: Hierarchy of assumptions.

Unit-2: H-atom Problem

Cartesian and polar coordinates. Center of mass and relative coordinates. General forms of solutions and orbital specifications. Spherical harmonics. Real and complex orbitals. Role of constant motion.

Unit-3: Group Theory 1

Reducible and irreducible representations, Classes and Characters, Great Orthogonality theorem and related theorem, Projection operators, Direct product representation, Construction of SALC, Selection rules in spectroscopy, Study of normal modes, IR and Raman activity.

Unit-4: Statistical Thermodynamics

Entropy and probability. MB distribution. Partition functions. Relevance to thermodynamics. PF for atoms and diatomics. Application to chemical/ionization equilibrium, Equipartition principle. Gibbs paradox and quantum statistics. Blackbody radiation.

Unit-5: Biophysical Chemistry

Configuration and conformation of biological macromolecules. Membrane structure. Spectroscopic methods : UV-Vis and CD. Separation techniques : Gel Electrophoresis. Macromolecule-ligand binding and cooperativity.

Course ID: CHEM - G 24

Practical Chemistry 2

Qualitative analysis of mixture of compounds.

Organic preparations.

Experiments (Kinetics, equilibrium, electrochemistry, spectroscopy)

SUGGESTED BOOKS FOR SEMESTERS I and II

Course ID: CHEM-G11 and CHEM-G21

Advanced Inorganic Chemistry - F. A. Cotton & G. Wilkinson

Inorganic Chemistry - J. E. Huheey, E. A. Keiter & R. L. Keiter

Chemistry of the Elements – N. N. Greenwood & A. Earnshaw

An Introduction to Inorganic Chemistry – K. L. Purcell & J. C. Kotz

Concepts and Models in Inorganic Chemistry – Douglass, McDanniel & Alexander

Coordination Chemistry – S. F. A. Kettle

Valence Theory – S. F. A. Kettle, J. N. Murrall & S. Teddler
Valence – C. A. Coulson

Chemical Application of Group Theory – F.A.Cotton

Theoretical Approach to Inorganic Chemistry – A. Williams

Inorganic Chemistry – D. F. Shriver, P. W. Atkins & C. H. Langford

Instrumental Methods of Analysis – Williard, Meritt, Dean & Sett

Electroanalytical Chemistry –A. J. Bard

Electrochemical Techniques for Inorganic Chemistry – J. B. Headri

Comprehensive Coordination Chemistry - G. Wilkinson, R. A. Gillard & J. A. McCleverty (eds)

Inorganic Chemistry –A. G. Sharpe

Inorganic Chemistry – Modern Introduction – T. Moeller

Supramolecular Chemistry - Jean-Marie Lehn Supramolecular

Chemistry Series - Edited by Jean-Mari Lehn

Self-Assembly in Supramolecular Systems - L. F. Lindoy and I. M. Atkinson

Vogel's Textbook of Quantitative Chemical Analysis - G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney

Analytical Chemistry – G.D. Christian

Fundamentals of Analytical Chemistry – D.A. Skoog, D.M. West and F.J. Holler

Nuclear and Radiochemistry- Friedlander, Kennedy and Miller

Essentials of Nuclear Chemistry – H.J. Arnikar

Nuclear Chemistry and its Application – Hossinsky

Bioinorganic Chemistry – R. W. Hay

Introduction to Bioinorganic Chemistry – D. R. Williams

Bioinorganic Chemistry –L. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine

General Principles of Biochemistry of Elements – E. I. Ochiai

Inorganic Aspects of biological and Organic Chemistry – R. P. Hanzlik

Principles of Bioinorganic Chemistry - , S. J. Lippard, J. M. Berg

Inorganic Chemistry of Biological Process – M. N. Hughes

An Introduction to Bioinorganic Chemistry – R. J. P. Williams

Organometallics A concise Introduction – Ch. Elschenbroich, A. Salzer

Inorganic Chemistry – Catherine E. Housecroft and A. G. Sharpe

Macrocyclic Chemistry, Current Trend and Future Perspectives – KarstenGloe

Organometallic Chemistry of transition Metals- R. H. Crabtree

Basic Organometallic Chemistry-B. D. Gupta & A. J. Elias

C. P. Horwitz& D. F. Shriver, *Advances in Organometallic Chemistry*, Vol. 23, 1984

Comprehensive Organometallic Chemistry- G. Wilkinson, F. G. A. Stone & E. W. Abel (Eds)

Electron Paramagnetic Resonance-Elementary Theory and Practical Applications- John A. Weil,
James R. Bolton & John E. Wertz

NigeiJ. Bunce; *Introduction to the Interpretation of Electron Spin Resonance Spectra of Organic Radicals*, *Journal of Chemical Education*, Vol. 64, 1987

Mossbauer Spectroscopy and Transition Metal Chemistry(Fundamentals and Applications)- Philipp
Guetlich, Eckhardt bill, A. X. Trautwein

Nuclear and Radiochemistry – Friedlander, Kennedy & Miller

Essentials of Nuclear Chemistry – H. J. Arnikar

Nuclear Chemistry – Williams

Nuclear Chemistry and its Applications – Hossinsky

Radiochemistry – A. N. Nesmeyanev

Radioactivity Applied to Chemistry – A. C. Wahl & N. A. Bonner

An Introduction to Radiation Chemistry – J. W. T. Spinks & R. J. Woods

(Course ID: CHEM–G12 and CHEM–G22)

Advanced Organic Chemistry - J. March.

Mechanism and Structure in Organic Chemistry - E. S. Gould.

Physical Organic Chemistry - J. Hine

Organic Chemistry - J. B. Hendrickson, D. J. Cram & J. H. Hammond.; 3rd edition.

Hammett equation - C. D. Johnson.

Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.

Stereochemistry of Organic Compounds - D. Nasipuri.

Pericyclic Chemistry - S. M. Mukherjee.

Orbital Symmetry - a Problem - solving approach.- R. E. Lehr and A. P. Marchand.

Orbital Symmetry in Organic Reactions - T. L. Gilchrist & R.C. Storr.

Organic Photochemistry - J. W. Coxon & B. Halton.

Elements of Organic Photochemistry - D. O. Cowan & K. L. Drisco.

Spectrometric Identification of Organic Compounds – R. M. Silverstein & F. O. Webster; 6th edition

Applications of Nuclear magnetic Resonance Spectroscopy in Organic Chemistry L. M. Jackman.

NMR and Chemistry – J. W. Akitt.

Organic Spectroscopy – W. Kemp, 3rd Edn.

Organic Synthesis - The Disconnection Approach – S. Warren

Designing Organic Synthesis – S. Warren

Tactics of Organic Synthesis - T.-L. Ho.

Exercise in Synthetic Organic Chemistry - C. Ghiron & R. J. Thomas.

Hydroboration - H. C. Brown

Borane Reagents - H. C. Brown, A. Pelter, K. Smith.

Radical Chemistry – M. J. Perkins.

Heterocyclic Chemistry - J. A. Joule & K. Mills.

Heterocycles in Synthesis – A. I. Meyers.

Organic Chemistry, Vol. II - I.L. Finar.

Natural Products – A. Pelter.

The Alkaloid- S. W. Pelletier

The Alkaloids - G. F. Cordell.

Relevant parts from Natural Products; Vols. I & II - P. S. Kalsi.

Relevant parts from Advanced Organic Chemistry - F.A. Carey and R.J. Sandberg; Vols. I & II.

Relevant parts from Comprehensive Organic Synthesis - B. M.Trost & I. Fleming.

Relevant parts from Comprehensive Heterocyclic Chemistry- A.R. Katritzky.

COURSE ID I CHEM-G13 and CHEM-G23

Physical Chemistry : A Molecular Approach – D.A. McQuarrie, J.D. Simon

Physical Chemistry – R.S.Berry, S.A.Rice, J.Ross

Introduction to Atomic Spectra – H.E. White

Quantum Mechanics- J.L.Powell, B. Crasemann

Introduction to Quantum Mechanics- D. J. Griffiths

Introduction to Quantum Mechanics – L.Pauling, E.B.Wilson

Quantum Chemistry – I.N.Levine

Coulson's Valence- R. McWeeny

Chemical Application of Group Theory- F. A. Cotton

Group theory and chemistry- D. M. Bishop

Chemical Kinetics – K.J.Laidler

Foundations of Chemical Kinetics – S.W. Benson

Theoretical Chemistry – S.Glasstone

Fundamentals of Statistical and Thermal Physics – F.Reif

Statistical Mechanics – R.K. Pathria

The Principles of Chemical Equilibrium – K. Denbigh

Thermodynamica and Introduction to Thermostatistics – H.B. Callen

Physics and Chemistry of Surfaces – N.K. Adams

Physical Chemistry of Surfaces – A.W. Adamson

Principles of Physical Biochemistry – K.V. van Holde, C. Johnson, P.S. Ho

Physical Chemistry of Macromolecules – C. Tanford

Polymer Chemistry – P.J. Flory

COURSE ID: CHEM-G14 and CHEM-G24

Practical Physical Chemistry – A.M. James, F.F. Prichard

Findlay's Practical Physical Chemistry – B.P. Levitt

Experimental Physical Chemistry – Shoemaker and Ga

SEMESTER – III

COURSE ID: CHEM-G31

Unit-1: IR, Raman, NMR and NQR spectroscopy of inorganic molecules

Applications of IR and Raman spectroscopy in inorganic chemistry (examples with organometallic, cluster and bioinorganic compounds). NMR spectroscopy of inorganic compounds: ^1H spectra of paramagnetic complexes, dipolar and contact shifts, magnetic susceptibility and resonance shifts. ^{11}B , ^{13}C , ^{19}F , ^{27}Al , ^{31}P NMR spectroscopy with typical examples. NQR spectroscopy: Principle, nuclear quadrupole coupling constant, structural information from NQR spectra.

Unit-2: PES and diffraction methods

Photoelectron spectroscopy: photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differentiation of same element in different environments from XPS, information about the nature of molecular orbital from UPS, UPS of simple diatomic molecules, e. g., N_2 , O_2 , CO , HCl , etc. Principles of electron, neutron and X-ray diffraction methods in determining the structure of molecules – a comparative approach.

Unit-3: Mass Spectroscopy

Principles, instrumentation and applications of mass spectrometry. Methods of generation of ions in EI, CI, FD and FAB and other techniques. Detection of ions, ion analysis, ion abundance, molecular

ion peak, metastable peak, isotopes, ion-molecule interaction and analysis of fragmentation patterns. Applications of mass spectroscopy to simple structural and mechanistic problems.

Unit-4: Absorption spectroscopy

L-B's Law and its limitations, Einstein's two level transition model. Transition moment and its relation to molar extinction coefficient. Different types of transitions ($\pi\pi^*$, $\sigma\pi^*$, $n\pi^*$ etc.), Selection rules with symmetry arguments, Solvent perturbation method, Weak and CT transition, Vibronic and spin orbit coupling.

Unit-5: Emission spectroscopy

Basic principle and instrumentation, FC principle, Mirror-image symmetry and its violation, Radiative and radiationless deactivation, Polarization characteristics of emission, Fluorescence Quenching (static and Dynamics), Fluorescence lifetime measurement.

CBCS PAPER

CBCS CHEM (50 marks, credit 04)

Unit-1: Environmental Chemistry (10 marks, 10 lecture-hours)

Environmental Hazards and Green Chemistry

Environmental Hazards and Pollution (their sources and remedies),

Green Chemistry-definition, need for Green Chemistry, limitations in the pursuit of Green Chemistry, basic principles, Applications of Green Chemistry to Chemical Synthesis.

Unit-II: Organometallic Chemistry and Catalyses (10 marks, 10 lecture hours)

(a) Organometallic Chemistry

Definition of organometallic compounds. Brief history. Concept of hapticity of organic ligands. 18-electron and 16-electron rules. Applications of 18-electron rule to metal carbonyls. General methods of preparation of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls. pi-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination and insertion reactions.

(b) Catalysis by Organometallic Compounds

Definition and importance of catalyst with special emphasis on Organometallic catalysts. Use of Organometallic catalysts with reference to industrially important processes.

Unit-3: Absorption and Emission spectroscopy (10 marks, 10 lecture hours)

Basic principle, instrumentation and application of absorption and emission spectroscopy (atomic and molecular): Fundamental Laws of photometry, Limitation of absorption and emission measurement, Photometric titration, Fluorescence quenching (Static and Dynamic), Time resolved measurement, Qualitative and quantitative analysis.

Unit-4: Nanoscience (10 marks, 10 lecture hours)

Introduction to nanoworld, Fundamental theories of nanoparticles (NPs), 0D, 1D and 2D nanoparticles and their physical, optical, electronic, magnetic properties, Methods of fabrication of metal organic and composite NPs, Application of NPs, nanoelectronics and devices.

Unit-5: Analytical Methods (10 marks, 10 lecture hours)

Basic Principles and Applications:

Optical spectroscopy for chemical analysis, Atomic Absorption Spectrometry,

Radiochemical Analysis, Electrochemical Analysis: Voltammetry, Thermogravimetric Analysis

SPECIAL PRACTICAL (THIRD SEMESTER)

CHEM SA-31

Practical Analytical Chemistry:

1. Environmental Analysis: Sampling and analysis of air/water/soil. Analysis of drug samples.
2. Physico-chemical experiments.
3. Quantitative estimation of alloys, ores and minerals.

CHEM SI-31

Practical Inorganic Chemistry:

1. Quantitative estimation of alloys and ores.
2. Physicochemical experiments.
3. Syntheses and characterization of coordination compounds.

CHEM SO-31

Practical Organic Chemistry

1. Chromatographic separation and identification of the components of a binary mixture of organic solids, mixture of organic liquids
2. Organic Preparation I
3. Organic Preparation II

CHEM-SP-31

Computer programming

SEMESTER – IV

Course ID: CHEM-SA41

Unit-1: Statistical Analysis of Data

Nature of error - systematic & random error; Random walk problem and probabilistic treatment of random errors; Confidence Intervals and Confidence Levels; Least square method for calibration plots; Regression and Correlation analysis.

Unit-2: Principles of Polymer Chemistry

Molecular weights and molecular weight distributions and their determinations (viscometry, osmometry, light scattering, size-exclusion chromatography; Principles of macromolecular synthesis: step-growth vs. chain-growth polymerizations.

Advanced synthetic techniques for controlling molecular weight dispersity in synthetic polymers- Living polymerization (living ionic, living radical and living ring-opening polymerizations); block copolymers-synthesis, microstructure, and applications; Conjugated polymers and their electrical and opto-electronic properties.

Unit-3: Advanced Techniques in Microscopy

Electron Microscopy - Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM); Atomic Force Microscopy (AFM); Fluorescence Confocal Microscopy; Fluorescence Correlation Spectroscopy.

Unit-4: Instrumentation and Application of Absorption & Emission Spectroscopy

Basic instrumentation for UV-VIS and IR spectroscopy – radiation source, Optical dispersive system, Detectors. Atomic Absorption Spectrometry – Radiation sources, different type atomizers, background correction, application.

Fluorescence and Phosphorescence: Structural factors, Photoluminescence Power as related to concentration, Instrumentation, Fluorescence Life time measurements. Room Temperature Phosphorescence, comparison of Luminescence and UV Absorption Methods.

Atomic emission spectroscopy: Instrumentation, Typical application, ICP Atomic Fluorescence Spectroscopy, comparison of Methods: ICP verses AAS.

Unit-5: Electrochemical Analysis

Non-faradic and faradic circuits; Electrode Processes – Diffusion controlled current under different initial conditions; Butler-Volmer equation and its Limiting Forms; Polarographic Techniques and Voltammetry and their various applications.

Course ID: CHEM-SI41

Unit – 1: Chemical application of Group Theory

Splitting of orbitals and free-ion terms in various environments; Correlation diagrams; Tanabe-Sugano diagrams; Metal centered spectral transitions (d-d and f-f) – selection rules, vibronic coupling, polarization, spectral parameters; Utilization of group theory in molecular orbital description; Charge transfer transitions.

Unit – 2: Varieties of inorganic and metallo-organic systems

Varieties of organic and inorganic ligands based on number and types of donor atoms, acyclic/cyclic nature, diamagnetic/paramagnetic property, σ/π -donor/acceptor aspect, strong-field/weak-field aspect, etc.); Metal ion specific ligands; Thermodynamic and kinetic aspects; Varieties and metal compounds; Geometries of the coordination environment; Design of ligands and metal compounds to get targeted properties (e. g. structural, magnetic, spectroscopic, electrochemical, catalytic, biomimetic, sensing, gas storage, superconducting, etc.); Uncertainties in predicting the composition and structure; Characterization and studies; Structure-property correlations; Important and path-breaking discoveries; Recent scenario and trends in national and international level.

Unit – 3: Solid state chemistry

Defects in solids, point, line and plane defects, determination of equilibrium concentration of Schottky and Frenkel defects, stoichiometric imbalance in crystals and non-stoichiometric phases, colour centres in ionic crystals, band theory, band gap, metals, insulators, semiconductors (intrinsic and extrinsic), hopping semiconductors, rectifiers and transistors, bonding in metal crystals, free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, superconductivity, Meissner effect, basic concept of BCS (Bardeen- Cooper- Schriffer) theory.

Unit – 4: Inorganic rings and clusters

Metal-metal bonding (MO approach), metal-metal single and multiple bonded compounds. Bonding in dimolybdenum and dirhenium complexes. Synthesis, structure, reactions and bonding as applicable in respect of molybdenum blue, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red. Iso- and hetero-polyoxometalates of V, Mo and W: synthesis, structure, reactions and uses. Low nuclearity (M_3 , M_4) and high nuclearity (M_5 - M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, capping rules, carbide, nitride, chalcogenide and halide containing clusters. Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

Unit – 5: Chemistry of f block elements

Terrestrial abundance and distribution; relativistic effect, oxidation states; aqueous, redox and complex chemistry in different oxidation states as applicable. Preparations, isolation, purification, properties and reactivities of the lanthanide and actinide elements and variations within the lanthanide and actinide series; lanthanide and actinide contraction and consequences; separation of lanthanides and actinides. Lanthanide compounds as high temperature superconductor, NMR shift reagent and MRI reagent. Organometallic compounds of lanthanides.

Course ID: CHEM-SO41

Unit-1: Stereochemistry-II

Advanced course involving conformation and reactivity- acyclic system, bicyclic systems, tricyclic systems.

Chiroptical properties of organic molecules, CD, ORD-principles and applications, haloketone rules, sector rules. Chiral analysis by Polarimeter, NMR, GC, HPLC and

Capillary Electrophoresis (CE) methods. Baldwin's Rules-applications, hydrolytic kinetic resolution.

Unit-2: Asymmetric Synthesis

Enantio- and diastereoselective synthesis. Reactions of enolates (□□ substitution), Addition to C=C double bonds (electrophile induced cyclisation, iodolactonisation, Conjugate additions. Reduction of C=C double bonds, Aldol Reaction, Diels Alder Cycloaddition, Cyclopropanation, Oxidation, Epoxidation, dihydroxylation and aminohydroxylation; Rearrangement: [3,3]-Sigmatropic, (2,3)-Wittig, alkene isomerisation.

Unit-3: Heterocyclic Chemistry-II

Nomenclature of fused heterocycles. Reactivity and synthesis of pyrimidine, pyridazines, pyrazines, purines, pteridines with and without oxygen and/or sulfur atoms, and their role in biological systems. Introduction to the chemistry of seven-membered heterocyclic compounds: azepines, oxepines, thiepinines and their aza-analogues.

Unit-4: Organometallic Chemistry of Transitional Elements

Application of organotransition metals in organic synthesis-preparative, structural and mechanistic aspects. Davies rule, catalytic nucleophilic addition and substitution reaction, Coupling reaction-Heck, Stille, Suzuki coupling Ziegler Naata reaction, Olefin metathesis, Tebbe's reagent, Pauson-Khand reactions, Volhsrdt co-trimerisation, functional organometallic compounds. Use of nontransition metal Indium, tin, zinc.

Unit-5: Medicinal Chemistry-I

Antibiotics – Penicillins, Cephalosporins, tetracyclins, newer generation of antibiotics. Chemistry of porphyrins

Pharmacodynamics - different types of drugs and drug targets, drug binding forces, role

Of enzymes. Drug – receptor interactions, mechanism of drug action, agonists,

antagonists. Affinity, efficacy and potency of a drug, dose-response curves.

Pharmacokinetics - drug absorption, distribution, metabolism (Phase-I and Phase-II

transformations), excretion, drug formulation and others.

COURSE ID: CHEM-SP41

Unit-1: Quantum Mechanics 2

Stern-Gerlach expt., Hilbert space, Dirac notation, Generalized uncertainty principle, position and momentum space rep. Continuous vs discrete basis, Delta function and Fourier transformation, Pictures- Schrodinger-Heisenberg-Dirac.

Unit-2: Quantum Mechanics 3

Time ordering, Dyson series upto second order correction, Fermi-Golden rule, Einstein A, B coefficient, Rabi oscillation, Sudden approximation. Gell-Mann and Low theorem. Symmetry in quantum mechanics, Parity and time reversal.

Unit-3: Perturbation Theory

Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications. Brillouin-Wigner theory. Matrix perturbation. Degenerate perturbation theory-Stark effect. First and second order lifting of degeneracy.

Unit-4: Quantum Chemistry 1

Variation method: Basis and applicability. Linear variation method- secular determinant. Many-electron systems: Closed and open shells, Antisymmetric principle and antisymmetrizer operator. Independent particle model (IPM). Self-consistent fields: Hartree and Hartree-Fock(HF) Theories. HF methods for closed shells. Implementation of HF method for closed shells: Roothaan equation. HF theory and Koopmans' theorem. Problems with open-shell systems. Restricted and unrestricted HF methods (elementary idea).

Unit-5: Quantum Chemistry 2

Electron correlation. Multideterminantal wave function and CI. Brillouin's theorem. Non-variational non-perturbative approximate methods- elementary exposure.

Rudiments of Density Functional Theory: Expectation Value calculation using density: Kohn-Hohenberg Theorems; Kohn-Sham equation for the ground state of many body systems; Fermi and Coulomb holes; exchange correlation functional.

COURSE ID: CHEM-SA42

Unit-1: Fundamentals of Chemical Analysis

Aim of analytical chemistry. Standardization and calibration. Quality assurance and quality control. Process control and validation.

Classical methods of analysis: Gravimetry and titrimetry including neutralization, complexation and oxidation-reduction. Complex acid-base equilibrium. Separation of metal ions as their hydroxides, sulphides and chelates. Examples of gravimetric and complexometric analysis.

Unit-2: Solvent Extraction and Concept of Chromatography

Liquid-Liquid extraction – Cross and counter current process, multiple batch extraction, solvent extraction of metal ion, solid-phase extraction. Classification of chromatographic separation. Aqueous biphasic and supercritical fluid extraction. Band broadening and column efficiency, Theoretical plate model and the Rate theory of Chromatography.

Unit-3: Liquid Chromatography and Other Types of Chromatography:

Reverse and normal phase chromatography, gradient elution, solvent selection and classes, ion exchange and ion chromatography.

HPLC: Basic equipment, pumping and injection system, column stationary phase and structural types of column packing, Detector systems (UV, IR, Conductometric, Fluorescence), Sample preparation and applications.

Gas chromatography: gas-liquid and gas-solid chromatography, types of column and selection. Basic equipment, Injection systems, Detectors (FID, TCD, ECD, NPD) for GC, sample separation and applications.

Characteristics and applications of Size exclusion Chromatography, Affinity chromatography, Supercritical Fluid Chromatography, Capillary Electrophoresis.

Unit- 4: Kinetics in Analytical Chemistry & Thermal Analysis

Significance of reaction kinetics in analytical chemistry. Determination of rate of fast reactions. Analytical application of catalytic and non-catalytic reactions in single species and pseudo single species systems. Differential reaction rate methods of analysis and its limitations, determination of inorganic and organic mixtures.

Principle, Instrumentation and application of TG, DTA, DSC and other Thermal Analysis Techniques. Factors affecting the Thermal Analysis Curves.

Unit-5: NMR Spectroscopy

Spin resonance. g Values and resonance frequencies for different nuclei. Larmor precession, relaxation times, chemical shift, coupling constant. Simplification of complex spectra: shift reagents, double resonance, NOE, spin tickling. NMR of nuclei other than ^1H (e.g. ^{13}C , ^{31}P , ^{19}F , ^{29}Si , ^{103}Rh , ^{129}Xe , ^{195}Pt , ^{11}B etc.). Integration and quantitative analysis. Spectra and Molecular Structure.

COURSE ID: CHEM-SI42

Unit – 1: Magnetochemistry

Definition of magnetic properties, types of magnetic bodies, experimental determination of magnetic susceptibility: Gouy method, Faraday method, vibrating sample magnetometer, SQUID, NR method. Anisotropy in magnetic susceptibility. Diamagnetism in atoms and polyatomic systems, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, Curie equation, Curie's law, Curie-Weise law, van Vleck equation and its application, Bleaney Bowers equation, first order and second order Zeeman effects, temperature independent paramagnetism, magnetic properties of transition metal complexes in cubic and axially symmetric crystal fields, low spin-high spin cross-over, magnetic behaviour of lanthanides and actinides, magnetic exchange interactions, Heisenberg-Dirac-van Vleck equation and its applications, magnetic materials.

Unit – 2: Crystallography

Crystal and lattice, process of crystallizations, crystal form, habit, defect, lattice planes, indices, crystal systems and symmetry, primitive and nonprimitive lattice, diffraction of X-ray, Brag's condition, reciprocal lattice, Brag's law in reciprocal lattice, Ewald sphere, X-ray Crystallography Instrumentation, goniometer, geometric data collection, crystal mosaicity and beam divergence, completeness of data collection, crystal to detector distance vs resolution, atomic scattering factor, structure factor, intensity of diffracted beam, Friedel's Law, systematic absences, temperature factor on the intensity of diffracted beam.

Unit – 3: Inorganic Reaction Mechanism

Introduction, Different types of reactions, Four broad classes of mechanism of substitution---“D”, “A”, “I_a” and “I_d”; Mechanism of substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to dⁿ ion complexes; Solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation; Mechanism of isomerization reaction---linkage isomerism, cis-trans isomerisms, intermolecular and intramolecular racemization; trans and cis effect and trans influence; Mechanism of electron transfer reactions: outer sphere and Inner sphere reactions.

Unit – 4: Supramolecular chemistry of inorganic molecules

Terrestrial abundance and distribution; relativistic effect, oxidation states; aqueous, redox and complex chemistry in different oxidation states as applicable. Preparations, isolation, purification, properties and reactivities of the lanthanide and actinide elements and variations within the lanthanide and actinide series; lanthanide and actinide contraction and consequences; separation of lanthanides and actinides. Lanthanide compounds as high temperature superconductor, NMR shift reagent and MRI reagent. Organometallic compounds of lanthanides.

Unit – 5: Selected topics on the chemistry of d block elements

Electronic configuration, common and unusual oxidation states, aqueous, redox and coordination chemistry of 3d, 4d and 5d elements. Conformational changes and thermochromism of Ni(II), Co(II) and other recently reported compounds. Mixed valence compounds of Fe, Cu, Pt, Fe-S compounds. Dinitrogen and dioxygen complexes of transition metals, Crutz-Taube complex, Vaska's complex.

Course ID: CHEM-SO42

Unit-1: NMR Spectroscopy-II

NMR shift reagents and their applications, basic two-dimensional sequence.

Application of ^1H - ^1H COSY, ^1H - ^{13}C HETCOR, HMBC, HMQC, HSQC, TOCSY, NOESY in structure elucidation of organic compounds, reaction monitoring etc., Solid state NMR (^{13}C -CP-MAS), Chemical Shift Anisotropy and Cross Polarisation, MRI as a diagnostic tool.

Unit-2: Bio-organic Chemistry

Molecular models of biological receptors, biomimetic chemistry, design, synthesis and binding studies of synthetic receptors. Enzyme models, micelles, polymers, cyclodextrins, remote functionalization reactions, catalytic antibodies, principle of gene synthesis. Proteins, peptides & amino acids.

Unit-3: Medicinal Chemistry -II

Drug design and synthesis, Molecular and quantum mechanics; Drawing chemical structures, equations, and diagrams; 3D structures; Molecular modelling and Energy Minimization; Molecular properties, Conformational analysis, Docking Procedures, *De novo* design, Molecular Recognition, Receptor Based Molecular Modeling, QSAR studies, Antineoplastic agents, cardiovascular drugs, Local anti-infective drugs, Antimalarial, Antibiotics, Anticholinergic and CNS-active drugs.

Unit-4: Carbohydrate Chemistry

Basic structure and type of sugars. Protection and deprotection. Deoxy-sugars, amino sugars, glycol sugars and their synthetic aspects. Synthetic approach (Combinatorial) towards polysaccharides of biological and industrial importance. Carbohydrates as chiral pools in organic synthesis.

Unit-5: Homo or Heteroatomic bond activation and functionalization: Metallic or non-metallic approach

Mechanisms of C-H bond activation with transition metals: Oxidative addition, sigma bond metathesis, electrophilic and metalloradical activation. Organic synthesis involving chelation-assisted C-H activation, *ortho*-C-H activation, C-H activation in heterocycles and base-assisted C-H activation. C-H, C=C and C≡C activated annulation reactions. Important synthetic approaches *via* C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis.

COURSE ID: CHEM-SP42

Unit-1: Kinetics 2

Rate processes and some physical phenomena. Statistical approach to rate theory: Hinshelwood, RRK and RRKM theories.

Unit-2: FT-NMR Spectroscopy

Introduction to pulsed-FT-NMR. Product-operator formalism of 1D and 2D NMR. Determination of three-dimensional structure of molecules using NMR spectroscopy.

Unit-3: Statistical Mechanics 1

Phase space, ergodic hypothesis, Liouville's theorem, Concepts of different ensembles with applications to selective systems. Fluctuations. Perfect gas and the Sackur-Tetrode equation, System of interacting molecules, treatment of imperfect gases.

Unit-4: Statistical Mechanics 2

Formulation of Quantum statistical mechanics: pure and mixed states, density matrix, quantum Liouville theorem and its consequences, Quantum statistics and ensembles. The specific heat of electron gas, Debye theory, Bose condensation.

Unit-5: Mathematical concepts

Elements of calculus, Extremum principles, constrained extremization, Power series: Convergence and divergence, Taylor series and Fourier series. Vectors and linear vector space: matrices. Applications.

COURSE ID: CHEM-SA43

Unit-1: Nuclear Models & Chemistry of Superheavy Elements

Nuclear models – Nuclear forces, liquid drop model, shell model, Magic numbers. Nuclear spin and nuclear isomerism. Nuclear reactions – energetics, mechanism and models, nuclear fission and nuclear fusion. Nuclear reactors and particle accelerators. Interaction of radiation with matter.

Production and nuclear properties of transactinide elements. Fundamental and experimental aspects of one-atom-at a time chemistry, gas phase and liquid phase chemistry, methods of their estimation.

Unit-2: Bioanalytical Methods & Forensic Analysis

Adulterated chemicals, explosives and pattern recognition. Forensic medicine – post-mortem and antemortem analysis, Narcotic drugs and psychotropic substances. Toxicology – poisons and venoms, Measurement of toxicity and toxicants, Drugs toxicity, Food toxicity.

Serology and DNA finger printing, Immunoassay – radio immunoassay of hormones, Fluoro immunoassay, Enzyme immunoassay,. Biosensors – cell based biosensors, electrochemical methods and biosensors, thermoionic, bioptical and piezoelectric biosensors.

Unit-3: Atmospheric Chemistry and Air Pollution

Characteristics of the atmosphere, radiation balance in the atmosphere, contribution of trace gases to Green House Effect. Atmospheric stability and meteorology. Gas phase atmospheric chemistry of N, S and volatile organic compounds, Photochemical smog and Acid rain. Particles in the

troposphere. Air pollutants – their source and effect, abatement and control. Chemistry of unperturbed and perturbed stratosphere–Antarctic Ozone Hole and Chlorofluorocarbons. Monitoring and determination of atmospheric gases and particles. Indoor air-pollution.

Unit-4: Environmental Chemistry of Hydrosphere & Lithosphere

Natural Water Systems: Composition, model system, residence time, treatment. Aquatic biochemical process, microorganism, kinetics of bacterial growth, microbial transportation of carbon, biodegradation of organic matters. Industrial and municipal waste water treatment. Principle of surface water quality modeling and control. Hydrological cycle, natural nutrients in aquatic ecosystem, eutrophication, oxygen and aquatic life, water pollution.

Environment chemistry of C, S, N, P and some biologically important metals. Pesticides, Organic pollutants and inorganic pollutants. Polymers and Plastics and their environmental degradation. Weathering of crustal rock and formation of soil. Soil temperature and heat transfer. Determination of C, N, K, P in soil.

Unit-5: Materials chemistry and nanochemistry

Classification of materials, semiconducting materials, organic soft materials, ceramics, composites, material characterization techniques, correlation between materials structure and their properties, structure and properties of technologically important crystalline and amorphous materials, recent breakthroughs in materials chemistry, synthesis and characterization of nanomaterials, properties and applications of nanomaterials.

COURSE ID: CHEM-SI43

Unit – 1: Advanced Inorganic Spectroscopy

Plane polarized light, CD, ORD and MCD spectra. Experimental aspects of absolute configuration of coordination compounds: Flack parameter. Cotton effect and Faraday effect, stereoselective and stereospecific effects. Advanced EPR spectroscopy and Mossbauer spectroscopy.

Unit – 2: Bioinorganic chemistry -2

Dioxygen storage/transport proteins: haemoglobin, myoglobin, hemerythrin and hemocyanin. Di-nitrogen fixation. Electron transport proteins: cytochromes, Fe-S proteins and other electron carrier

proteins in biology. Metalloproteins catalysing oxygen atom transfer reaction: iron containing enzymes such as methane monooxygenase, nitric oxide reductase; Molybdenum containing enzymes such as xanthine, sulphite oxidase and nitrate, trimethylamine-N-oxide, DMSO reductase. Other selected metalloproteins of various metal ions. Structure/function analogue of above mentioned systems.

Unit – 3: Organometallic chemistry – 2

Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples.

Catalysis by organometallic compounds: Hydrogenation of unsaturated compounds, Wilkinson's catalyst, Tolman catalytic loop; Syntheses gas- water gas Shift reaction; Hydroformylation (oxo process); Monsanto acetic acid process; Wacker process, synthetic gasoline-Fischer-Tropsch process and Mobile process; polymerization, oligomerization and metathesis reaction of alkenes and alkynes, Ziegler-Natta catalysis, photodehydrogenation catalyst (platinum POP).

Unit – 4: Sensing of Analytes

Preamble, Jablonski diagram, photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, substitution, fragmentation, isomerisation, exchange and redox reactions; chemiluminescence, photochromism; determination of quantum yield, inorganic photochemistry in biological processes and their model studies; applications of photochemical reactions of coordination compounds - synthesis and catalysis, solar energy conversion and storage, sensing of biologically relevant cations and anions: chemosensors and chemodosimeters.

Unit – 5: Materials chemistry and Nanochemistry

Classification of materials, semiconducting materials, organic soft materials, ceramics, composites, material characterization techniques, correlation between materials structure and their properties, structure and properties of technologically important crystalline and amorphous materials, recent breakthroughs in materials chemistry, synthesis and characterization of nanomaterials, properties and applications of nanomaterials.

Course ID: CHEM-SO43

Unit-1: Nanoscience and Organic Electronics

Basic concept on nanoparticles, quantum dot and nanocluster, surface atom effect, quantum size effect, non-metal to metal transition, special properties of nanoparticles, important routes for fabrication of nanoparticles and porous nanomaterial, method of characterization, their application as smart catalyst in organic synthesis (e.g. C-C, C-N, C-O coupling reactions under reductive and oxidative conditions), Fabrication of J- and Haggregates with organic compounds, their characterization and development of their optoelectronic properties. Designing organic electronic devices such as OFET, OLED, solar cell etc. and their efficiency as high-tech devices.

Unit-2: Green Chemistry and Supramolecular Chemistry

Green chemistry- overview, Twelve Principles, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave. Solvent free organic reactions.

From molecular to supramolecular chemistry: factors leading to strong binding (non-covalent interactions). New molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes.

Unit-3: Nucleoside & Nucleotide

Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Amino-acids-protein biosynthesis. Covalent interactions of nucleic acids with small molecules. Structural features of DNA and RNA.

Unit-4: Natural Products as Lead Drug

Synthesis and mechanism of, anti-tumor, antiviral, anti-sense and DNA cleaving agents.

Unit-5: Advanced Organic Synthesis

Key Ring Forming Reactions: Robinson Annulation, Intramolecular Nucleophilic Alkylation, Intramolecular Michael Reaction, Cation-Olefin Cyclization, Anionic Cyclization, Nazarov Cyclization, Divinylcyclopropane Rearrangement, Oxy-Ene Reaction (Conia Reaction), Cyclopentanone Annulation Methodology, Pauson-Khand Reaction, Carbonylation Cyclization, Olefin Ring Closing Metathesis.

COURSE ID: CHEM-SP43

Unit-1: Solids

Reciprocal lattice, Structure factor, Fourier synthesis, Band theory, band gap, metals and semiconductors –intrinsic and extrinsic semiconductors, superconductors.

Unit-2: Group Theory 2

MO theory with applications to σ and σ^* bonding and construction of hybrid orbitals. LFT with applications to splitting of terms and levels in different coordination environments and construction of energy level diagrams, Applications of symmetry principles in Woodward-Hoffman type reactions like dimerization of ethylene and Diels-Alder reaction.

Unit-3: Quantum Mechanics 4

Harmonic oscillator (wavefunction and operator methods), Coherent state, Constants of motion. Representations. Commutation relations. Step up/down operators. Quantization. Spin and Pauli matrices. Matrix representations of total angular momentum operators. Many electron systems.

Unit-4: Principle of Lasers and its applications

Two level transition (absorption, induced and stimulated emission), Einstein model for two levels transition, Principle of Maser and Laser action. Population inversion (two/three/four level systems), Basic element in laser (resonator, Gain medium, Pumping technique), Characteristics of laser radiation (coherence: temporal/spatial; polarization, monochromaticity, intensity), Single mode laser (solid/ gas laser: Ruby, Nd:YAG, Ar-ion, CO₂, Excimer etc.) tunable laser (Dye laser), Harmonic generation, Application of laser (chemical problem, medicinal and industrial).

Unit-5: Theoretical Spectroscopy

Selection rule for vibrational spectra, anharmonic correction by perturbation - appearance of overtones, selection rule for rotational spectra, nuclear spin and energy levels, Stark effect, Raman scattering, selection rule for rotation-vibrational Raman effect. Nonlinear scattering- hyper-Raman, Stimulated and Resonance Raman spectra.

SUGGESTED BOOKS for SEMESTERS III & IV

COURSE ID: CHEM-G31, CBCS, CHEM-SA41, CHEM-SA42, CHEM-SA43

Vogel's Textbook of Quantitative Chemical Analysis - Jeffery, Bassett, Mendham and Denney

Analytical Chemistry – G.D. Christian

Fundamentals of Analytical Chemistry – D.A. Skoog, D.M. West and F.J. Holler

Instrumental Methods of Chemical Analysis – G.W. Ewing

Instrumental Methods of Analysis – H.H. Willard, L.L. Meritt, J.A. Dean and F.A. Settle

Treatise on Comprehensive Analytical Chemistry – Wilson and Wilson

The mathematics for Physics and Chemistry(Vil-1)- H. Marganau and G.M. Murphy

Mathematical Methods in Chemistry – Mackie, T.M. Shephard and C.A. Vincent

Mathematics for Chemists – D.M. Hirst

Statistics for Analytical Chemistry – J.C. Miller and J.N. Miller

Nuclear and Radiochemistry- Friedlander, Kennedy and Miller

Essentials of Nuclear Chemistry – H.J. Arnikar

Nuclear Chemistry and its Application - Hossinsky

Electrochemical Methods – A.J. Bard and L.R. Raukner

Electroanalytical Chemistry – H.W. Nurnberg (Ed)
Electroanalytical Chemistry- A.J. Bard
Electroanalytical Techniques for Inorganic Analysis – J. B. Headridge
Radiochemistry – A. N. Nesmeyanov
Radioactivity applied to chemistry – A. C. Wahs and N. A. Bonner (Ed)
An introduction to Radiation chemistry – J. W. T. Spinks and R. J. Woods
Non-aqueous Solvents – L. F. Audrieth
Non-aqueous Solvents – T. C. Waddington
Atomic Absorption Spectrometry – B. Welz
Atomic Absorption Spectrometry –J. W. Robinson
Analytical Chemistry, Principles – J. H. Kennedy
Analytical Chemistry, Principles and Techniques – L. G. Hargis
Chemical Separation Methods – J. A. Dean
Solvents Extraction of chelates – Morrison and Freiser
Practical Clinical Biochemistry – A. H. Gowenlock
Toxicological Chemistry – Vora
Environmental Toxicology, Ed. J. Rose
Environmental Chemistry – A. K. De
Environmental Chemistry – C. Baireid, W. H. Freeman
The Chemistry of our Environment – R. A. Horn
Environmental Chemistry, An Introduction – L. I. Pryde
Electron Microscopy, J.J. Bozzola, L.D. Russell
A Manual of Applied Techniques for Biological Electron Microscopy, Michael J Dykstra
Atomic Force Microscopy: Understanding the Basic Modes and Advanced Applications,
Greg Haugstad
Confocal Microscopy Methods and Protocols, Ed.: Stephen W. Paddock
Fundamentals of Light Microscopy and Electronic Imaging, Doulgas B. Murphy
Single Molecule Spectroscopy, R. Rigler, M. Orrit, T. Basche
Handbook of Single Molecule Fluorescence Spectroscopy, C Gell, D. Brockwell, A. Smith
Principles of Fluorescence Spectroscopy, J. Lakowicz
Principles of Polymer Chemistry, P.J. Flory
Semiconducting and Metallic Polymers, A.J. Heeger
Fundamentals of Polymer Science – An Introductory Text, M.M. Coleman & P.C. Painter
The Hydrophobic Effect : Formation of Micelles and Biological Membranes, C. Tanford

Polymer Chemistry: An Introduction, M.P. Stevens

Fundamentals of Polymerization, B.M. Mandal

The Chemistry of Polymers, J.N. Nicholson

Polymers in Solution: Their Modelling and Structure, J. Cloizeaux & G. Zanninu

Nucleic Acids, S. Doonan

Biophysical Chemistry of Proteins (An Introduction to Laboratory Methods), E. Buxbaum

Introduction to Materials Chemistry by Harry R. Allcock, John Wiley and Sons

Materials Chemistry by Bradley D. Fahlman, Springer.

Nanomaterials and Nanochemistry by Catherine Brechignac and Philippe Houdy, Springer.

Nanochemistry by Kenneth Klabunde Gleb Sergeev, Elsevier.

COURSE ID: CHEM-G31, CBCS, CHEM-SI41, CHEM-SI42, CHEM-SI43

Chemical Application of Group Theory – F. A. Cotton Group Theory
and chemistry – D. M. Bishop

Electron Paramagnetic Resonance – Elementary Theory and

Practical Applications – John A. Weil, James R. Bolton & John E. Wertz

Introduction to Ligand Fields – B. N. Figgis

Introduction to Ligand Fields Theory – C. J. Ballhausen Valence

- C. A. Coulson

Chemical Crystallography – L. W. Bunn Crystal

& X-ray – K. Lansdale

Crystal Structure Analysis – M. J. Buerger X-ray

Crystal Structure – D. Melachlan Elements of X-ray

Crystallography - Azaroff

Introduction to Metal – Complex Chemistry – M. Tsutsui Modern

Inorganic Chemistry – J. J. Lagowski Introduction to Solids –

Azaroff

Solid State Physics – A. J. Dekker Principle

of Solid state – H. V. Kevv

Ionic Crystal Lattice & Non-Stoichiometry – N. N. Greenwood Solid

State Chemistry – N. B. Hannay

Solid State Chemistry & Its Application – A. R. West

Symmetry in Molecules – J. M. Hollar

Advanced Inorganic Chemistry – F. A. Cotton & G. Wilkinson

Inorganic Chemistry – J. E. Huheey, E. A. Keiter & R. L. Keiter

Comprehensive Coordination Chemistry – G. Wilkinson, R. D. Gillard & J.A. McCleverty Inorganic
Reaction Mechanism – M. L. Tobe

Mechanism of Inorganic Reaction – F. Basolo & R. G. Pearson

Mechanism of Inorganic Reaction – Katakis & Gordon Chemistry of
Complex Equilibria – M. T. Beck & V. I. Nagypal Treatise on Analytical
Chemistry – Kolthoff Elving

Photochemistry of Coordination Compounds – V. Balazani & V. Carassiti Determination
and use of Stability Constants – A. E. Martell & R. J. Motekaitis Critical Stability
Constants – A. E. Martell

Chemistry – S. F. A. Kettle

Principle and Applications of Organotransition Metal Chemistry J. P.
Collman, L. S. Hegehus & R. G. Finke

Magnetochemistry – A. Selwood Introduction to
Magnetochemistry Earnshaw

Physical Methods in Inorganic Chemistry – R. S. Drago

Physical Methods in Advanced Inorganic Chemistry – H. A. O. Hiel & P. Day Concepts of
Inorganic Photochemistry – A. W. Adamson & P. D. Fleishauer Magnetic Resonance
Spectroscopy – R. M. L. Bell & R. K. Harris

Comprehensive Coordination Chemistry – G. Wilkinson, R. D. Gillard & E.
W. Abel (Eds.)

Bioinorganic Chemistry – R. W. Hay

Introduction to Bioinorganic Chemistry – D. R. Williams

Bioinorganic Chemistry – L. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine

General Principles of Biochemistry of Elements – E. I. Ochiai

Inorganic Aspects of biological and Organic Chemistry – R. P. Hanzlik

Principles of Bioinorganic Chemistry - , S. J. Lippard, J. M. Berg

Inorganic Chemistry of Biological Process – M. N. Hughes

An Introduction to Bioinorganic Chemistry – R. J. P. Williams

Comprehensive Organometallic Chemistry – G. Wilkinson, F. G. A. Stone & E. W. Abel (Eds.)

Organo Transition metal Chemistry – S. G. Davies

Organometallic Chemistry of Transition Metals – R. H. Crabtree

Ions in Biological Systems – H. Siegel (Ed.)

An Introduction to Inorganic Chemistry – K. F. Purcell & J. C. Kotz

Elements of Magnetochemistry – R. L. Dutta & A. Shyamal Principles of Organometallic Chemistry – R. L. Crabtree Homogeneous Catalysis; Wiley: New York, 1980

G. W. Parshall Heterogeneous Catalysis

Applied Homogeneous Catalysis with Organometallic Compounds – W. A. Herrmann Catalyst Handbook – B. B. Pearce

Homogeneous Catalysis - G. W. Parshall and S. D. Ittel

Applied Homogeneous Catalysis with Organometallic Compounds – B. Cornils & W. A. Herrmann

S. P. Sinha, Ed., Lanthanide & Actinide Research (Journal, Vol. 1, 1986)

The Chemistry of Actinide Elements, Vols. 1 & 2 - J. J. Katz, G. T. Seaborg and L. R. Morss

Kinetics and Mechanism of Reaction of Transition Metal Complexes - R. G. Wilkins X-RAY Structure Determination – A Practical Guide-George H. Stout and Lyle H. Jensen Structure Determination by X-ray Crystallography, MFC Ladd and R. A. Palmer

Crystal Structure Analysis for Chemists and Biologists, Jenny P. Glusker with Michell Lewis
Miriam Rossi

Crystal Structure Analysis for Chemists and Biologists - Jenny P. Glusker, Mitchell Lewis, Miriam Rossi

Crystal & X-ray – K. Lansdale

Crystal Structure Analysis – M. J. Buerger

X-ray Crystal Structure – D. Melachlan

Elements of X-ray Crystallography –Azaroff

Advance Inorganic Chemistry- F. A. Cotton & G. Wilkinson

Chemistry of Elements – N. N. Greenwood & Earnshaw

Inorganic Chemistry – Catherine E. Housecroft and A. G. Sharpe

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COURSE ID: CHEM-G31, CBCS, CHEM-SO41, CHEM-SO42, CHEM-SO43

Advanced Organic Chemistry - J. March.

Physical Organic Chemistry – J. Hine.

Organic Chemistry - J. B. Hendrickson, D. J. Cram & J. H. Hammond; 3rd edition.

Organic Chemistry – J. Clayden; N. Greeves; S. Warren & P. Wothers.

Organic Reaction Mechanics- A. Gallego, M.Gomer & Sierra, M.A

Physical Organic Chemistry - N. S. Isaacs - Longman.

Hammett equation - C. P. Johnson.

Symmetry in Chemistry - Orchin & Jaffe.

Symmetry Rules in Chemical Reactions - R. G. Pearson.

Orbital Interactions in Chemistry - T. A. Albright, J. K. Burdt & M. H. Whangbo.

Pericyclic Chemistry - S. M. Mukherjee.

Orbital Symmetry - a Problem - solving approach.- R. E. Lehr and A. P. Marchand.

Orbital Symmetry and Organic Reactions - T. L. Gilchrist & R. C. Storr.

Conservation of Orbital Symmetry – R. B. Woodward & R. Hoffman

Pericyclic Reactions; Vols. I & II - R.E. Lehr & A. P. Marchand.

Frontier Orbitals and properties of Molecules - V. F. Tranen.

Huckel M.O. Theory - K. Yates.

Frontier Orbitals and Organic Chemical Reactions - I. Fleming.

Pericyclic Chemistry - Gill & Willis.

Strained Organic Molecules – A. Greenberg & J. F. Liebman.

Organic Photochemistry - J. W. Coxon & B. Halton.

Elements of Organic Photochemistry - D. O. Cowan & K. L. Drisco.

A Handbook of Computational Chemistry - Tim Clark.

Radical Chemistry – M. J. Perkins.

Free Radicals in Organic Chemistry - J. Fossey, D. Lepost & J. Sorba.

Hammett Equation - C. D. Johnson.

Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.

Stereochemistry of Organic Compounds - D. Nasipuri.

Applications of Nuclear magnetic Resonance Spectroscopy in Organic Chemistry L. M. Jackman.

NMR in Chemistry - A Multinuclear Approach - W. Kemp.

Pulse & Fourier Transform NMR - T. C. Farrar & E. D. Becker.

The Nuclear Overhauser Effect in Structural & Conformational Analysis - D. Neuhaus.

Modern NMR Techniques for Chemistry Research - A. E. Derome.

NMR: The Toolkit – P. J. Hore; J. A. Jones & S. Wimperis

Two-dimensional Nuclear Magnetic Resonance in Liquids - A. Bax.

Interpretation of Carbon-13 NMR spectra - F. W. Wehrli & T. W. Wirthlin.

Introduction to Mass Spectrometry - S.R. Shrader, A. B. Bacon.

Mass Spectroscopy - Organic Applications - K. Biemann.

Mass Spectrometry - K.G. Das

Modern Organic Reactions - H.O. House – Benjamin

Principles of Organic Synthesis - R.O.C. Norman and J. M. Coxon-Blackie.

Some Modern Methods of Organic Synthesis - W. Carruthers – Cambridge University Press.

Application of Organotransition Metals in Organic Synthesis - S.G. Davies.

Principles and Applications of Organotransition Metal Chemistry – J. P. Collman, L. S. Hegedus, J. R. Norton & R. C. Finke.

Organotransition Metal Chemistry – R. F. Heck.

Synthetic Coordination and Organometallic Chemistry- A. D. & Kharisov, B. I.

Palladium in Organic Synthesis – Tsuji, J.

Palladium in Heterocyclic Chemistry: A Guide for the Synthetic Chemist- Li, J. J. & Gribble, G.W.

Supramolecular Chemistry - Concepts and Perspectives - J. -M. Lehn

Principles and Methods in Supramolecular Chemistry – Schneider, H.-J; Yatsimirski

Current Trends IN Organic Synthesis – Scolastico, C. & Nicotra, F.

Organic Synthesis - The Disconnection Approach - Stuart Warren

Designing Organic Synthesis - Stuart Warren

Tactics of Organic Synthesis - T.-L. Ho.

Exercise in Synthetic Organic Chemistry - C. Ghiron & R. J. Thomas.

Hydroboration - H. C. Brown

Borane Reagents - H.C. Brown, A. Pelter & K. Smith.

Radical Chemistry - M. J. Perkins.

Modern Methods in Carbohydrate Synthesis – Khan, S. H.; O’Neil, R. A.

The Chemistry of Sugar – Levy, D. E.; Fugedi, P.

Glycoscience: Chemistry and Chemical Biology- Fraser-Reid, B. O.; Tatsuta, K.;

Thiem, J.

Heterocyclic Chemistry - J. A. Joule & K. Mills.

Heterocycles in Synthesis – A. I. Meyers.

Organic Chemistry, V I. - I. L. Finar.

Natural Products: Chemistry, and Biological Significance - J. Mann; R. S. Davidson,

J.B. Hobbs, D.V. Banthorpe; J.B. Harbome & Longman, E.

Organic Chemistry- Vol. II. I. L. Finar.

Relevant portions from -Chemistry of Alkaloids- edtd. By RH.F.

Manske; Academic Press.

The Alkaloids - J.A. Cordell.

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New Trends in Natural Product Chemistry - Atta-ur-Rahaman and M. I. Choudhury,
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Relevant portions from Burger's Medicinal Chemistry and Drug Discovery; Ed. M. E.
Wolff, John Wiley.

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Press.

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Synthesis of Organic Medicinal Compounds – Ishar, M. P. S. & Faruk, A.

Fundamentals of Medicinal Chemistry -Thomas; G.

Classics in Total Synthesis by K. C. Nicolaou & E. J. Sorenson

Introduction to Medicinal Chemistry - A. Gringuage; Willey-VCR.

An Introduction to Medicinal Chemistry – G.L. Patrick, 3rd Edn

Instant Notes: Medicinal Chemistry- Patrick G.

Handbook of Anticancer Drug Development – Budman, D. R.; Calvert, A. H. and
Rowinsky, E. K.

Surface and Nanomolecular Catalysis – R. Richards

The Nanoscope Encyclopdia of Nanoscience & Nanotechnology, Vol-I to VI; Diwan
P. & Bharadwaj, A.

Microwave Assisted Synthesis of heterocycles – R. R. Gupta; V. E. Eric & Kappe, C.
Oliver

Microwaves in Organic and Medicinal Chemistry –Kappe;C: Oliver & Stadler

New Trends in Green Chemistry- V. K. Ahluwalia & M. Kidwai.

Solvent-free Organic Synthesis – K. Tanka

Green Chemistry - V. K. Ahluwalia

Green Chemistry – P. T. Anastas & T. C. Williamson

COURSE ID:CHEM-SO31

A Textbook of Practical Organic Chemistry - A.I. Vogel.

Qualitative Organic Analysis - A.I. Vogel.

Quantitative Analysis - A.I. Vogel.

An Introduction to Experimental Organic Chemistry - Roberts,

Gilbert, Rodewald & Wingrove.

Handbook of Organic Analysis - H.T. Clarke.

Systematic Qualitative Organic Analysis- H. Middleton.

Thin Layer Chromatography - Egon Stahl.

Spectrometric Identification of Organic Compounds – R. M. Silverstein & F. O.

Webster; 6th edition

COURSE ID: CHEM-G31, CBCS, CHEM-SP41, CHEM-SP42, CHEM-SP43

Introduction to Quantum Mechanics- D. J. Griffiths

Quantum Mechanics- J.L.Powell, B. Crasemann

Molecular Quantum Mechanics- P.W.Atkins

The Feynman Lecturers in Physics, Vol. 3- R. P. Feynman, R.B. Leighton, M. Sands

Modern Quantum Chemistry- A. Szabo, S. N. Ostlund

Elementary Quantum Chemistry- F. L. Pilar

Quantum Chemistry- I. N. Levine

Coulson's Valence- R. McWeeny

Chemical Application of Group Theory- F. A. Cotton

Group theory and chemistry- D. M. Bishop

Thermodynamics and introduction to Thermostatistics- H. B. Callen

Element of classical thermodynamics- A. B. Pippard

Theories of chemical reaction rates- K. J. Laidler

Theory of rate processes – S. Glasstone, K. J. Laidler, H. Eyring

Fundamentals of Molecular Spectroscopy – C.W. Banwell

Fundamentals of Molecular Spectroscopy – G.M. Barrow

Molecular spectroscopy- I. N. Levine

Molecular Spectroscopy – J. D. Graybeal

Principle of Fluorescence Spectroscopy- J. R. Lakowicz

Modern Spectroscopy – J.M. Hollas

Symmetry and Spectroscopy – D.C. Harris, M.D. Bertolucci

Molecular Vibrations – E.B. Wilson Jr., J.C. Decius, P.C. Cross

Laser Spectroscopy – W. Demtroder

Statistical and Thermal Physics- F. Reif

Statistical Mechanics- D. A. McQuarrie

Statistical Mechanics – S. K. Ma

Statistical Mechanics- K. Huang

Statistical Mechanics- R. K. Pathria

Statistical Mechanics- B. B. Laud

Chemical Kinetics and Dynamics- J. I. Steinfeld, J. S. Francisco, W. L. Hase

Molecular reaction dynamics - R. D. Levine

Molecular reaction dynamics and chemical reactivity- R. D. Levine, R.B. Bernstein

Introduction to Solid State Physics – C. Kittel

Introduction to Solid State Theory – O.Madelung

Solid State Physics – N.W. Ashcroft, N.D. Mermin

Solid State Physics – A.J. Dekker

Advanced Engineering Mathematics – E. Kreyszig

Mathematical Methods in the Physical Sciences – M.L. Boas

COURSE ID: CHEM-SP31

Programming with Fortran – S. Lepschutz, A.Poe

Numerical Recipes in Fortran, The Art of Scientific Computing – W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery

CBCS CHEM (50 marks, credit 04)

UNIT-I

Environmental Chemistry (10 marks, 10 lecture-hours)

Environmental Hazards and Green Chemistry
Environmental Hazards and Pollution (their sources and remedies),
Green Chemistry-definition, need for Green Chemistry, limitations in the pursuit of Green Chemistry, basic principles, Applications of Green Chemistry to Chemical Synthesis.

UNIT-II

Organometallic Chemistry and Catalyses (10 marks, 10 lecture hours)

(c) Organometallic Chemistry

Definition of organometallic compounds. Brief history. Concept of hapticity of organic ligands. 18-electron and 16-electron rules. Applications of 18-electron rule to metal carbonyls. General methods of preparation of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls. pi-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination and insertion reactions.

(d) Catalysis by Organometallic Compounds

Definition and importance of catalyst with special emphasis on Organometallic catalysts. Use of Organometallic catalysts with reference to industrially important processes.

UNIT-III

Absorption and Emission spectroscopy (10 marks, 10 lecture hours)

Basic principle, instrumentation and application of absorption and emission spectroscopy (atomic and molecular): Fundamental Laws of photometry, Limitation of absorption and emission measurement, Photometric titration, Fluorescence quenching (Static and Dynamic), Time resolved measurement, Qualitative and quantitative analysis.

UNIT-IV

Nanoscience (10 marks, 10 lecture hours)

Introduction to nanoworld, Fundamental theories of nanoparticles (NPs), 0D, 1D and 2D nanoparticles and their physical, optical, electronic, magnetic properties, Methods of fabrication of metal organic and composite NPs, Application of NPs, nanoelectronics and devices.

UNIT-V

Analytical Methods (10 marks, 10 lecture hours)

Basic Principles and Applications:

Optical spectroscopy for chemical analysis, Atomic Absorption Spectrometry, Radiochemical Analysis, Electrochemical Analysis: Voltammetry, Thermogravimetric Analysis

REFERENCE BOOKS:

1. Environmental Chemistry – C. Baired, W. H. Freeman
2. The Chemistry of our Environment – R. A. Horn
3. New Trends in Green Chemistry- V. K. Ahluwalia & M. Kidwai

4. Solvent-free Organic Synthesis – K. Tanka
5. Green Chemistry - V. K. Ahluwalia
6. Green Chemistry – P. T. Anastas & T. C. Williamson
7. Principles of Organometallic Chemistry, Chapman and Hall, 1988-P. Powall
8. Principles and Applications of Organo transition Metal Chemistry. Mill Valley, CA: University Science Books, 1987- J. P. Collman, et al.
9. The Organometallic Chemistry of the Transition Metals. New York, NY: John Wiley, 2000- R. H. Crabtree.
10. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006- J. E. Huheey, , E.A. Keiter & R.L. Keiter.
11. Advanced Inorganic Chemistry 6th Ed. 1999., Wiley. F.A. Cotton, G. Wilkinson, C. A. Murrillo, M. Bochmann.
12. Nanoscopic Materials – Size Dependent Phenomena by Emil Roduner
13. Self-Assembly and Nanotechnology – A Force Balance Approach by Yoon S. Lee
14. Fundamentals of Molecular Spectroscopy – C.W. Banwell
15. Introduction to Molecular Spectroscopy – G.M. Barrow
16. Fundamentals of Photochemistry – K.K. Rohatgi-Mukherjee
17. Molecular Spectroscopy – I.N. Levine
18. Principles of Fluorescence Spectroscopy, Joseph R. Lakowicz
19. Analytical Chemistry – G. D. Christian
20. Fundamentals of Analytical Chemistry – D. A. Skoog, D. M. West and F. J. Holler
21. Radiochemistry and Nuclear Methods of Analysis – William D. Ehmann, Diane E. Vance
22. Treatise on Comprehensive Analytical Chemistry – Wilson and Wilson
23. Introduction to Thermal Analysis: Techniques and Application – M. E. Brown

