SYLLABUS

FOR

TWO-YEAR FOUR-SEMESTER COURSE IN

CHEMISTRY

2014

UNIVERSITY OF CALCUTTA

DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALCUTTA

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

COURSE STRUCTURE

Duration	S E M E S T E R								Total Marks
	I July - Dec		II Jan - June		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	-	-	-	550
*Special (S)					100	100	150	100	450
Total Marks	150	100	150	100	150	100	150	100	1000

*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	
	Theo	Pract
CHEM – G11	50	-
CHEM – G12	50	-
CHEM – G13	50	-
CHEM – G14	-	100
Total	150	100

SEMESTER – II (Marks – 250)

Course ID	Marks	
	Theo	Pract
CHEM – G21	50	-
CHEM – G22	50	-
CHEM – G23	50	-
CHEM – G24	-	100
Total	150	100

SEMESTER – III (Marks – 250)

Course ID	Marks	
	Theo	Pract
***CHEM – G31**	50	-
****CHEM – SA32/SI32/SO32/SP32**	50	-
****CHEM – SA33/SI33/SO33/SP33**	50	-
****CHEM – SA34/SI34/SO34/SP34**	-	100
Total	150	100

*General (G): Compulsory

**One Special course to be opted and continued systematically

SEMESTER – IV (Marks – 250)

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

*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 – SA34/SI34/SO34/SP34	50	50	-

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

Course ID	Grand viva	$Continuous assessment	Write-up, Oral presentation and discussion
*CHEM – SA44/SI44/SO44/SP44	20	40	40

*Project work, throughout the practical hours of the semester; topic should be outside the UG/PG curriculum of CU; use of LCD projector is mandatory; time 20 m, followed by discussion

$To be assessed by the guide

SYLLABUS

Semester – I

Course ID: CHEM–G11

Unit-1: Symmetry
Symmetry elements and symmetry operations. Group theory. Group multiplication tables and molecular point groups. Platonic solids. Stereographic projections of point groups. Introduction of periodic symmetry.

Unit-2: Coordination Chemistry 1
Crystal field theory. Splitting of d-orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral 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. 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. Limits of applicability of crystal field theory. Shapes of complexes.

Unit-3: Bioinorganic Chemistry 1
Elements of life: basic reactions in biological systems and roles of metal ions. Bioenergetic principle and role of ATP. Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin. Transport across biological membrane: Na^{+}-K^{+}-ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxy peptidase, urease. Metal dependent disease: Wilson's disease, Alzheimer disease. Metal complexes as drugs: Pt, Rh, Ru and Au drugs. Toxic effects of metal ions, detoxification by chelation therapy.

Unit-4: Solid-state Chemistry 1
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.

Unit-5: Electrochemical Analyses
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 aromaticty, annulenes, heteroannulenes, fullerenes (C_{60}), 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 1
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**
Classification and stereochemical modes. Thermal and photopericyclic reactions, Selection rules and stereochemistry of electrocyclic reactions, 2-component cycloadditions, sigmatropic rearrangements, carbene addition. Rationalization based on Frontier M.O. approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Sommelet, Hauser, Cope and Claisen rearrangements, Ene reaction, Wittig rearrangement.

Unit-4: NMR Spectroscopy 1
Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant(J), spin decoupling, spin tickling, classification of 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.

Unit-5: Natural Products 1 – Terpenoids
Isoprene rule, Structure elucidation (by chemical and spectroscopical methods), Synthesis, Biogenesis and Biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes. Structural types: general introduction to sesqui-, di- and tri-terpenoids.

Course ID: CHEM-G13

Unit-1: Thermodynamics
State functions. Legendre transformation. Caratheodory's theorem and principle. Applications. Thermodynamics of phase transitions.

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 tunnelling.

Unit-4: Kinetics 1
Fast reactions. Oscillatory reactions. Autocatalysis. Electrode kinetics: Nernst, Butler-Volmer and Tafel equations.

Unit-5: Absorption Spectroscopy
$\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ and $d \rightarrow d$ transitions. Solvent effects. Weak and CT interactions. Vibronic and spin-orbit coupling.

Course ID: CHEM–G14

Practical Chemistry 1
Spectrophotometric, ion exchange and complexometric estimations.
Identification of single organic liquid with one or more functional groups.
Numerical, kinetic and equilibrium experiments.

Semester – II

Course ID: CHEM–G21

Unit-1: Chemical Bonding

Different types of bonding including weak interactions. Variation method. LCAO method. Molecular orbital of H_2^+, H_2, homo and hetero diatomic, triatomic and polyatomic molecules/ions (including T_d, O_h, and D_{4h} coordination complexes). Molecular term symbols. Electron pair wave function, VB theory and its application to H_2 molecule. Comparison of VB and MO theories.

Unit-2: Coordination Chemistry 2

Metal-centered electronic spectra of transition metal complexes: microstates, determination of ground and all excited state terms of d^n ions, splitting of d^n terms in octahedral and tetrahedral fields, Orgel diagrams (qualitative approach), hole formalism – inversion and equivalence relations, selection rule for spectral transitions, d-d spectra and crystal field parameters, nephelauxetic series. Qualitative idea of Tanabe-sugano diagrams, Charge transfer spectra. Magnetic properties of coordination compounds: spin and orbital moment, spin-orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable-temperature magnetic moments.

Unit-3: Organometallics 1

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, isolobal and isoelectronic relationships with examples. Metal-alkyl, -allyl, -carbene, -carbonyl, -carbide and cyclopentadienyl complexes. Structure and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_4H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$ and $[Co_2(CO)_6(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Unit-4: Chemistry of the Elements 1

Polymorphism of C, P and S. Structure and bonding in higher boranes based on Lipscomb's topological concept, Wade's rules, borohydride $B_nH_n^{2-}$ anions, carboranes, metalloboranes, hydroboration reactions. Alkali metal complexes with macrocyclic ligands (crown ethers, cryptates and spherand). Aqueous and complex chemistry of beryllium and aluminium, basic beryllium compounds. Main group organometallics: classification, syntheses, reactions, structure and bonding and applications of typical examples.

Unit-5: Statistical Error and Radiochemical Analyses

Errors in quantitative analyses, types of errors, handling of systematic errors. Random errors: distribution, standard deviation, confidential limits of the mean, presentation of results, propagation of random errors.

Detection and measurement of radiation. Tracer techniques: study of chemical reactions, nuclear medicine. Nuclear activation analyses. Charged particle activation analyses.

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 1
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: Heterocyclic Chemistry 1
Synthesis and reactivity of pyridine, quinoline, isoquinoline, indole, pyrazole, imidazole, oxazole, thiazole, isooxazole and their applications in organic synthesis.

Unit-4: Synthetic Methodology 2
Organosulphur- Chemistry of organosulphur compounds, Sulphur- stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylides, chiral sulphoxides, umpolung
Nitrogen ylide, oxonium ylide

Unit-5: Natural Products 2 - Alkaloids
Familiarity with methods of structure elucidation (chemical & spectroscopical method), biosynthesis, synthesis and biological activity of alkaloids (nicotine, atropine, coniine and papaverine).

Course ID: CHEM - G23

Unit-1: Quantum Mechanics 2
Bound-states. Box with finite walls; the Kronig-Penney model and formation of bands. Harmonic oscillator (wavefunction and operator methods). Elements of variational method and perturbation theory.

Unit-2: The H-atom Problem
Cartesian and polar coordinates. Centre of mass and relative coordinates. General forms of solutions and orbital specifications. Spherical harmonics. Real and complex orbitals. Role of constants of motion.

Unit-3: Kinetics 2
PE surface, reaction coordinates and reaction paths. BEBO method. Absolute rate theory. Sample case-studies. Comparison with collision theory. Ionic reactions in solutions.

Unit-4: Statistical Thermodynamics
Entropy and probability. MB distribution. Partition function. Relevance to thermodynamics. PF for atoms and diatomics. Applications to chemical/ionization equilibrium. Equipartition principle. Gibbs paradox and quantum statistics. Blackbody radiation.

Unit-5: Interfacial Chemistry
Curved surfaces: Young-Laplace and Kelvin equations. Adsorption on solids: BET equation. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; micro- and macro-emulsions.

Course ID: CHEM - G24

Practical Chemistry 2
Qualitative analyses of mixture of inorganic compounds.
Organic preparations.
Instrumental experiments and computer programming.

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. F. Williams
Bioinorganic Chemistry – R. W. Hay
Introduction to Bioinorganic Chemistry – D. R. Williams
Elements of Bioinorganic Chemistry – G. N. Mukherjee & A. Das
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
Inorganic Chemistry –A. G. Sharpe
Inorganic Chemistry – Modern Introduction – T. Moeller
Supramolecular Chemistry - Jean-Marie Lehn
Supramolecular Chemistry Series - Edited by Jean-Marie 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
Radiochemistry and nuclear methods of analysis - William D. Ehmann, Diane E. Vance
Fundamentals of Analytical Chemistry – D.A. Skoog, D.M. West and F.J. Holler
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

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: 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 Quantum Mechanics – L. Pauling, E. B. Wilson
Quantum Mechanics – J. L. Powell, B. Crasemann
Quantum Chemistry – I. N. Levine
Chemical Kinetics – K. J. Laidler
Foundations of Chemical Kinetics – S.W. Benson
Fundamentals of Molecular Spectroscopy – C.W. Banwell
Introduction to Molecular Spectroscopy – G. M. Barrow
Theoretical Chemistry – S. Glasstone
Statistical and Thermal Physics – F. Reif
Statistical Mechanics – R. K. Pathria
The Principles of Chemical Equilibrium – K Denbigh
Thermodynamics and an Introduction to Thermostatics – H. B. Callen

The Physics and Chemistry of Surfaces – N. K. Adams
Physical Chemistry of Surfaces – A.W. Adamson

Course ID: CHEM–G14 and CHEM–G24

Macro and Semimicro qualitative Analysis – A. I. Vogel
Spot Tests in Inorganic Analysis – F. Feigel & V. Anger (translated by R. Oesper)
Quantitative Inorganic Analysis – A. I. Vogel
Quantitative Inorganic Analysis – G. Charlot & D. Bezier (translated by R. C. Murray)
Quantitative Chemical Analysis – I. M. Kolthoff, E. B. sandel, J. Meehan & S. Bruckenstein

Experimental Organic Chemistry - Principles & Practice - L.M. Harwood & C.J. Roodey
Qualitative Organic Analysis - A.I. Vogel
Text Book of Practical Organic Chemistry - A. I. Vogel
Hand Book of Organic Analysis - R.T. Clark
Systematic Qualitative Organic Analysis- H. Middleton.

Practical Physical Chemistry – A. M. James, F. F. Prichard
Findlay's Practical Physical Chemistry – B. P. Levitt
Experimental Physical Chemistry – Shoemaker and Garland
Computer Programming on Fortran IV – V. Rajaraman
Programming with Fortran – S. Lepschutz, A. Poe

Semester – III

Course ID: CHEM–G31

Unit-1: EPR and Mössbauer Spectra

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

Mössbauer activity: principle, experiment, line-width, center shift, quadrupole interaction, magnetic interaction; information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mössbauer active nuclei in varieties of environments.

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: Emission Spectroscopy

FC principle. Mirror-image symmetry and its violation. Radiative and radiationless deactivation. Polarization characteristics of emission. Quenchers and lifetime variations.

Unit-5: FT Spectroscopy

Advantages of time-domain vs. frequency-domain studies. Principles of FT-IR and pulse-FT-NMR with instrumentation.

Course ID: CHEM-SA32

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: Synthetic polymers and Biopolymers

Introduction to polymers - synthetic polymers, carbohydrates, proteins, and nucleic acids; 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.

Unit-3: Elements of Electronics and Instrumentation 1

Basic structure of chemical instruments. Transducers. Passive component and their properties. Semiconductor diods and transistors. Amplifier properties. Negative and positive feed back. Operational amplifiers. Oscillators. Power supplies.

Unit-4: Elements of Electronics and Instrumentation 2

Nonlinear and digital circuits – basic binary, logic gates counters, microprocessor, Application to specific chemical instruments.

Unit-5: Instrumentation and Application of Absorption 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.

Course ID: CHEM-SI32

Unit-1: Group Theory 1

Group theory and quantum mechanics (elementary ideas), representation of point groups, reducible and irreducible representations, definitions of classes and character, statement of Grand Orthogonality Theorem, construction of character table, reduction formula, direct product representation and its uses, symmetry of normal modes, normal mode analysis, selection rules for IR and Raman transitions. Hybridization.

Unit-2: Solid State Chemistry 2

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-Copper-Schriffer) theory, Application of DTA, DSC and TGA methods. X-ray diffraction analysis (spectral analysis, particle-size determination, etc.).

Unit-3: Organometallics 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 metatheses reaction of alkenes and alkynes, Ziegler-Natta catalysis, photodehydrogenation catalyst (platinum POP).

Unit-4: Bioinorganic Chemistry 2

Dioxygen transport/storage proteins: hemoglobin, myoglobin, hemerythrin and hemocyanin. Electron transport proteins: cytochromes, Fe–S proteins. Other electron carriers in biosystems. Respiratory electron transport chain. Photosynthesis, chlorophyll, PS-I, PS-II, photosynthetic electron transport chain. Nitrogen fixation. Cobalamins including vitamin and coenzyme B12.

Structural/functional models of some of the above-mentioned systems.

Unit-5: Inorganic Rings, Cages and Clusters

Metal-metal bonding (MO approach), metal-metal single and multiple bonded compounds. 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.

Course ID: CHEM-SO32

Unit-1: Stereochemistry 2

Advanced course involving conformation and reactivity- acyclic system, monocyclic systems- 3 to 10 member rings, 6-6, 6-5, 6-4, 5-5 bicyclic systems, 6-6-6, 6-5-6, 5-6-5, 5-5-5 tricyclic systems. Introductory course on molecular mechanics computations.

Unit-2: NMR Spectroscopy 2

Advanced Techniques and Applications of NMR: ^{1}H and ^{13}C NMR principles, rules for carbon 13 calculations, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation processes, population transfer, selective polarization transfer, NMR shift reagents and their applications, basic two-dimensional sequence.

Unit-3: Asymmetric Synthesis 1

Principles and newer method of asymmetric synthesis (including enzymatic and catalytic nexus), enantio- and diastereoselective synthesis. Reactions of enolates (α–substitution), Addition to C=C double bonds (electrophile induced cyclisation, iodolactonisation, Hydroboration, Conjugate additions.

Unit-4: Heterocyclic Chemistry 2
Nomenclature of bicyclic and tricyclic fused systems; Introduction to the chemistry of azepins, oxepins, thiepins and their aza-analogues; Phosphorus and selenium containing heterocycles. Cyclazines.

Unit-5: Medicinal Chemistry 1
Antibiotics – Penicillins, Cephalosporins, tetracyclins, newer generation of antibiotics. Chemistry of porphyrins, Lipids, Polyunsaturated fatty acids, Arachidonic acid cascade. Prostaglandins- structure & synthesis.

Course ID: CHEM-SP32

Unit-1: **Angular Momentum**
Constants of motion. Representations. Commutation relations. Step-up/step-down operators. Quantization. Spin and Pauli matrices. Matrix representations of total angular momentum operators. Many-electron systems.

Unit-2: Group theory 1
Reducible and irreducible representations; classes and characters; grand orthogonality theorem and related theorems; projection operators; direct product representation; construction of SALC; selection rules in spectroscopy; study of normal modes.

Unit-3: Valency
Born-Oppenheimer approximation and beyond. Avoided crossings. Virial theorem and chemical bonding. Theories of valence: VB and MO. Pi electron Hamiltonians: hierarchy of assumptions.

Unit-4: 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.

Unit-5: Kinetics 3
Rate processes and some physical phenomena. Statistical approach to rate theory: Hinshelwood, RRK and RRKM theories.

Course ID: CHEM-SA33

Unit-1: Fundamentals of Chemical Analysis
Aim of analytical chemistry. Sampling. Decomposition and dissolution of organic and inorganic samples. Elemental organic analysis. Quality assurance and quality control. Process control and validation.
Acid-base equilibrium aqueous and non-aqueous system. Separation of metal ions as their hydroxides, sulphides and chelates. Gravimetric analysis using organic reagents.

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: Complex Equilibrium
Stability of mono-nuclear, poly-nuclear mixed ligand complexes in solution. Determination of stability constants by potentiometric, spectrophotometric and polarographic methods. Conditional stability constant and application of complexometric titration in analytical chemistry.

Unit- 4: Kinetics in Analytical Chemistry
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.

Unit-5: Thermal Analysis
Principle, Instrumentation and application of TG, DTA, DSC and other Thermal Analysis Techniques. Factors affecting the Thermal Analysis Curves.

Course ID: CHEM–SI33

Unit-1: Crystallography 1
X-ray (related fundamentals), crystal forms, lattice, primitive cell, crystal systems and symmetry, non-primitive lattices, crystal classes, space groups, crystals and their proper ties, Diffraction of X-ray, lattice planes, indices, Brag's condition, reciprocal lattice, Bragg's law in reciprocal space.

Unit-2: Magnetochemistry 1
Definition of magnetic properties, types of magnetic bodies, experimental arrangements for determination of magnetic susceptibility: Gouy method, Faraday method, vibrating sample magnetometer, SQUID, NMR method. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic systems, Pascal's contants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, Curie equation, Curie's law and Curie-Weiss law.

Unit-3: Inorganic Reaction Mechanism
Mechanism of substitution reactions,: solvent exchange, aquation, anation, base hydrolysis, acid catalysed aquation, pseudo-substitution. Four broad classes of mechanism of substitution – 'D', 'A', 'Ia' and 'Id'. Mechanism of isomerization reaction – linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms.

Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non-mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Unit-4: Complex Equilibria 1

Thermodynamic and stoichiometric stability constants of metal-ligand complexes. Determination of composition and stability constants of complexes by pH-metric, spectrophotometric and polarographic methods. Conditional stability constants and their importance in complexometric EDTA titration of metal ions.

Unit-5: Chemistry of the Elements 2

Dinitrogen and dioxygen complexes of transition metals: syntheses, structures, bonding and reactivity.

Iso- and heteropolyoxometalates with respect of V, Mo and W: syntheses, reactions, structures, uses.

Metal-metal bonding (M.O. concept), metal-metal bonded dinuclear d-metal complexes-typical examples. Bonding in dirhenium complexes.

Syntheses, properties, reactions, structures and bonding as applicable in respect of molybdenum blues, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red, Crutz-Taube complex, Vaska's complex.

Course ID: CHEM-SO33

Unit-1: Applications of MO Theory

MO theory and its applications to organic molecules, Construction of MOs: linear and cyclic conjugated systems; *ab initio* methods. Walsh orbitals of cyclopropane and cyclobutane. Stability of carbocations, pi-facial selectivities, Cieplak model; strained organic molecules: calculation of strain energies; synthesis of strained cyclic molecules.

Unit-2: 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.

Unit-3: Synthetic Methodology 3

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

Unit-4: Medicinal Chemistry 2

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.

Unit-5: Natural Products 3
Steroids: General methods of study and structural types. Chemistry of cholesterol, hormones, bile acids, Vitamins of D-group, Diosgenin. Terpenoids: General study and structural features of sesquiterpenes, diterpenes, triterpenes; carotinoids; chemistry of representative members from the diterpenoid and triterpenoid series, carotenoids.

Course ID: CHEM-SP33

Unit-1: Biophysical chemistry
Structure and function of Biomolecules: Protein, nucleic acid, carbohydrates and lipids. Membrane structure. Biomolecular complexes: Protein – ligand, Enzyme – substrate and Drug – DNA. Examples. Techniques for study of biomolecular structure and function: Fluorescence and CD.

Unit-2: Electrochemistry
Debye-Huckel theory, Debye-Huckel-Onsager theory, Electrophoretic and relaxation effects, Wien effect, Debye–Fulkenhagen effect. Electrocapillarity (EC) – nature of EC curves, Lipmann equation. Helmholtz, Guoy-Chapman and Stern double layer models.

Unit-3: 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.

Unit-4: Vibration-rotation Spectra
Principles. Rotational Coherence Spectroscopy, Rotational and Vibrational spectra (electronic excitation: pump-probe technique) of excited and transient states. Time-resolved IR, 2-d IR, rotovibrational spectra.

Unit-5: NMR Spectroscopy 2
Product-Operator formalism of 1 D and 2D NMR. Coherence and polarization transfer experiments. Determination of three-dimensional structure of molecules using NMR spectroscopy.

Course ID: CHEM-SA34

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.

Course ID: CHEM-SI34

Practical Inorganic Chemistry:

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

Course ID: CHEM-SO34

Practical Organic Chemistry:

1. Chromatographic separation and identification of the components of a binary mixture of organic solids
2. Name-Reactions-Based Organic Preparations
3. Multistep Organic Preparations

Course ID: CHEM-SP34

Practical Physical Chemistry:

1. Selected analytical experiments.
2. Selected numerical experiments: algorithms and programming.
3. Selected instrumental experiments.

Semester - IV

Course ID: CHEM-SA41

Unit-1: Electrochemical Analysis

Introduction to non-faradic and faradic analysis. Non faradic method –High frequency titration. Faradic method – electrode kinetics, General feature of diffusion, Laplace transformation, Solution of diffusion equation under different initial conditions – Polarography, Tast method.

Unit-2: Advanced Topics in Polymer Chemistry

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: Nuclear Chemistry

Nuclear models – Nuclear forces, liquid drop model, Fermi gas 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.

Unit-4: Liquid Chromatography

Reverse and normal phase, 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.

Unit-5: Other Types of Chromatography

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

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

Course ID: CHEM-SI41

Unit-1: Group Theory 2

Splitting of orbitals and free ion terms in weak crystal fields, symmetries and multiplicities of energy levels in strong crystal fields, correlation diagram, Tanabe-Sugano diagram. Effect of lowering of symmetry on the orbitals and energy levels, correlation table. Justification of Laporte selection rule, vibronic coupling and vibronic polarization,

polarization of electronically allowed transitions. Symmetry adapted linear combinations (SALCs) and the M. O. description of organic, inorganic and organometallic molecules.

Unit-2: Crystallography 2
Geometric data collection (simple examples), structure factor, systematic absence, heavy atom method. Fourier synthesis, Patterson function, experimental diffraction methods (Laue method, rotating crystal method).

Unit-3: Bioinorganic chemistry 3
Metalloproteins catalyzing oxygen atom transfer reactions: Iron systems such as cytochrome P-450, methane monooxygenase, catechol and other dioxygenases, etc.; Molybdenum systems such as xanthine oxidase, sulphite oxidase, nitrate reductase, etc. Protective metalloenzymes such as superoxide dismutase, catalase and peroxidase. Other selected metalloproteins of various metal ions. Biological function of nonmetallic elements (other than C, H, O, N, S, P). Interaction of metal ions with bioligands.
Structural/functional models of some of the above mentioned systems.

Unit-4: Chemistry of the Elements 3
Nuclear stability, terrestrial abundance and distribution; relativistic effect, electronic configuration and oxidation states; aqueous, redox and complex chemistry in different oxidation states as applicable; electronic spectra and magnetic properties- comparisons with those of the d-block elements.
Preparations. Properties and reactivities of the lanthanide and actinides elements and variation within the lanthanide and actinide series; lanthanide and actinide contraction and consequences. Separation of lanthanides and actinides.

Unit-5: Nuclear Chemistry
Nuclear models – Nuclear forces, liquid drop model, Fermi gas 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.

Course ID: CHEM-SO41

Unit-1: Stereochemistry 3
Chiroptical properties of organic molecules, CD, ORD-principles and applications, haloketone rules, sector rules, helicity rules, exceptions and excitation chirality; atomic and conformational asymmetry. Chiral analysis by Polarimeter, NMR, GC, HPLC and Capillary Electrophoresis (CE) methods. Baldwin's Rules-applications, hydrolytic kinetic resolution.

Unit-2: Asymmetric Synthesis 2
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 3
Pyrimidines, pyridazines, pyrazines, purines, pteridines, compounds with oxygen and sulfur hetero atoms. Role of heterocyclic compounds in biological systems.

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: Supramolecular Chemistry
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. Supramolecular reactivity and catalysis, switching devices. self-assembly of supramolecular aggregates, crystal engineering.

Course ID: CHEM-SP41

Unit-1: Quantum mechanics 3
Coordinate, momentum and matrix representations. Pictures. Constant of motions. Virial, hypervirial and Hellmann-Feynman theorems; applications. Generalized uncertainty relation. Momentum eigenfunctions, delta function and Fourier transformation. Time reversal.

Unit-2: Perturbation theory
Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications. Brillouin-Wigner theory. Matrix perturbations. Degenerate perturbation theory – Stark effect. First and second order lifting of degeneracy.

Unit-3 : Time-dependent Quantum Processes
Perturbative dynamics. Semiclassical treatment of radiation-matter interaction – first order and second order effects. Golden rule. Einstein's A, B coefficients. Connection of results with experimental quantities. Two-level system.

Unit-4: Quantum Chemistry 1
Variation method : basis and applicability. Linear variation method – secular determinant. Many–electron systems: Closed and open shells. Antisymmetry principle and antisymmetrization operator. Independent particle model (IPM). Hartree and Hartree Fock methods for closed shells. Implementation of HF method for closed shells: Roothan equation.

Unit-5: Quantum Chemistry 2
HF theory and Koopman's theorem. Problems with open-shell systems. Restricted and unrestricted Hartree-Fock methods (elementary idea). Limitation of IPM: electron

correlation. Multideterminantal wave function and CI. Brillouin's theorem. Nonvariational-nonperturbative approximate methods – elementary exposure.

Course ID: CHEM-SA42

Unit–1: 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.

Unit-2: Bioanalytical Methods
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
Natural Water Systems: Composition, model system, residence time, treatment. Aquatic bio-chemical 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.

Unit-5: Environmental Chemistry of Lithosphere
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.

Course ID: CHEM – SI42

Unit-1: Spectroscopy 1
Survey of metal centered transitions of 3d, 4d, and 5d metal ion complexes. f-f spectra of lanthanides and actinides. Bonding parameters and structural evidences from electronic spectra. Charge transfer spectra. CD, ORD, and MCD spectra and absolute configuration

of coordination compounds. Cotton effect and Faraday effect, stereoselective and stereospecific effects.

Unit-2: Inorganic Photochemistry
Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing. Photochemical processes: photosubstitution and photoelectron transfer reactions in Co, Cr, and Rh complexes.

Unit-3: Complex Equilibria 2
Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes. Solubility equilibria: Quantitativeness of precipitation (of metal hydroxides, sulphides, and chelate complexes).

Unit-4: Magnetochemistry 2
First order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes in cubic and axially symmetric crystal fields, low spin-high spin crossover, magnetic behaviour of lanthanides and actinides, magnetic exchange interactions, magnetic materials.

Unit-5: Chemistry of the Elements 4
Electronic configuration, oxidation states, aqueous, redox and coordination chemistry, spectral and magnetic properties in different oxidation states, horizontal and vertical trends in respect of 3d, 4d and 5d elements with particular refernce to Ti-Zr-Hf, V-Nb-Ta, Cr-Mo-W, Mn-Tc-Re, Ru-Rh-Pd, Os-Ir-Pt.
Occurrence, isolation and purification in respect of V, Mo, W, Re; Pt group metals from Pt concentrate. Noble character of Pt group metals.

Course ID: CHEM-SO42

Unit-1: NMR Spectroscopy 3
Application of DEPT, ^{1}H-^{1}H COSY, ^{1}H-^{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.

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 3
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 dugs, Antimalarial, Antibiotics, Anticholenergic and CNS-active drugs.

Unit-4: Carbohydrate Chemistry
Basic structure and type of sugars. Protection and deprotection. Deoxy-sugars, amino sugars, glycal sugars and their synthetic aspects. Synthetic approach (Combinatorial) towards polysaccharides of biological and industrial importance. Carbohydrates as chiral pools in organic synthesis.

Unit-5: Natural Products 4
Structure, transformation and biosynthesis of alkaloids from terrestrial and marine sources; Chemistry of quinoline alkaloids with special reference to cinchona group; Chemistry of isoquinoline alkaloids – morphine group; Alkaloids derived from pyrrolidines and piperidine ring systems, and from ring systems containing two nitrogen atoms. Peptide alkaloids and Macrocyclic alkaloids.

Course ID: CHEM-SP42

Unit-1: Statistical Mechanics 1
Phase space; ergodic hypothesis; Liouville's theorem. Concepts of different ensembles with applications to selected systems. Fluctuations. Perfect gas and the Sackur-Tetrode equation. System of interacting molecules; treatment of imperfect gases.

Unit-2: 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-3: Mean field theories
Concept of a mean field: Thomas-Fermi model and Debye-Huckel theory.
Self-consistent fields: Hartree and Hartree-Fock theories. Rudiments of density functional theory: expectation value calculation using density; Kohn-Hohenberg theorems; Kohn-Sham equation for the ground states of many body systems. Fermi and Coulomb holes in density functional approach; meaning of exchange correlation functional.

Unit-4: Statistical Mechanics 3
Einstein's theory of Brownian motion, Langevin equation, Fokker-Planck equation, Fluctuation-dissipation relation, effect of friction. Applications to Kramer's theory and transport problems. Master equation and its applications.

Unit-5: Reaction Dynamics
Basic concepts in classical mechanics of collisions. Intermolecular potential from scattering experiments. Features of potential energy surfaces. Expermental methods. Study

of molecular energy transfer and state-to-state reactions. Macroscopic rate from microscopic rate coefficients.

Course ID: CHEM-SA43

Unit-1: NMR Spectrometer

Continuous–Wave NMR Spectrometers, Spectra and Molecular Structure. Elucidation of NMR Spectra–Double Resonance, NOE, Spin Tickling, Solvent Influence and Shift Reagents. Quantitative Analysis and Integration.

Unit-2: Instrumentation and Application of Emission Spectroscopy

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-3: Advanced Techniques in Microscopy

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

Unit-4: Chemistry of Superheavy Elements

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-5: Nanochemistry

Theoretical aspects; preparation, characterization, and applications of nanomaterials. Properties of nanomaterials and nanoparticles.

Course ID: CHEM-SI43

Unit-1: Spectroscopy 2

Application of IR, Raman, ESR, Mössbauer and PES in inorganic chemistry (examples with simple and complex inorganic compounds including organometallic and cluster compounds and bioinorganic systems).

NMR Spectroscopy: ^{1}H NMR spectra of paramagnetic coordination compounds, 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: Chemistry of the Elements 5

Compounds of Sc, Y, La, and Ac; Ce(III) and Ce(IV) compounds and their reaction. Lanthanide compounds as high temperature superconductor and nmr shift reagent and MRI reagent.
Isolation and purification of uranium from natural source; aqueous, redox and complex chemistry of uranium in different oxidation states, simple and complex uranium compounds-their preparation, properties, and reactions, organimetallic compounds of uranium. Transuranium and transactinium elements. Nuclear reactors and atomic energy, nuclear fuel reprocessing. Indian scenario.

Unit-3: Chemistry of the Elements 6
Chemistry of Ti, V, Mo, W, Re; Cu, Ag, Au in common and unusual oxidation states. Mixed valence compounds of Fe, Cu, Pt; Fe-S compounds, cobaloxime related compounds, conformational changes and thermochromism of Ni(II) compounds, Ru(II) and Ru(III) compounds, oxo compounds of Ru and Os, Rh(I) and Ir(I) carbonyl halide and carbonylhydrides.

Unit-4: Materials Chemistry 1
Syntheses, structures and bonding features and technical applications in respect of polymeric inorganic materials: polysilanes, polyoxysilanes, polyphosphazenes, polyphosphates, silicates, aluminosilicates with special reference to talc, mica, asbestos, zeolite, coordination polymers, dendritic macromolecules based on inorganic elements, Zintle phases, haliogen X_n^+ ions and their compounds, charge transfer complexes with halogens and halogen bridges or as ligands. Clathrates. Perxenic acid and its salts. Metal alkoxides and aryl oxides, metal complexes with oxo anions as ligands. One dimensional solids, solid state extended arrays, cheveral phases.

Unit-5: Nanochemistry
Theoretical aspects; preparation, characterization, and applications of nanomaterials. Properties of nanomaterials and nanoparticles.

Course ID: CHEM-SO43

Unit-1: Nanoscience and Organic Electronics
Basic concept on nanoparticles, quantum dot and nanocluster, surface atom effect, quantum size effect, nonmetal 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 H-aggregates 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
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.

Unit-3: Nucleoside and 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: Natural Products 5
Structure, transformations, synthesis of simple and monoterpenoid derived indole alkaloids – yohimbine, reserpine, strychnine, ellipticine, lysergic acid, representative examples of Iboga and Aspidosperma type indole alkaloids.

Course ID: CHEM-SP43

Unit-1: Solids
Reciprocal lattice. Structure factor. Fourier synthesis. Band theory, band gap. Metals and semiconductors – intrinsic and extrinsic semiconductors. Superconductivity.

Unit-2: Group Theory 2
MO theory with applications to σ and π 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: Chemistry of Excited States
Rotational, vibrational and electronic excited states. Excited state isomerisation reaction. Predissociation. State-specific predissociation and photofragmentation, excited state dynamics. Spectroscopy of cold molecules; single molecule spectroscopy.

Unit-4: Lasers
Principles of Maser and Laser action. Population inversion (two/three/four level systems). Basic elements in laser (resonator, Gain medium, Pumping technique). Characteristics of laser radiation (coherence: temporal/spatial; polarization, monochromaticity, intensity). Single mode and tunable laser. Harmonic generation. Applications. Optical birefringence.

Unit-5: Theoretical Spectroscopy
Selection rule for vibrational spectra, anharmonic correction by perturbation – appearance of overtones; selection rule for rotational spectra, nuclear spin and rotational energy levels, stark effect. Raman scattering, selection rule for rotational vibrational Raman effect. Non-linear scattering – hyper-Raman, stimulated Raman and resonance Raman spectra.

Suggested Books for Semesters III and IV

Course ID: CHEM-SA32, CHEM-SA33, 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(Vol-1)- H. Marganau and G.M. Murphy
Mathematical Methods in Chemistry – Mackie, T.M. Shephardand 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. Nesmeyanev
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
Basic Concepts of Analytical Chemistry- S. M. Khopkar
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. Baired, 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 … - 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. Buxbaun

Course ID: CHEM–SA34

Quantitative Inorganic Analysis – A. I. Vogel
Quantitative Inorganic Analysis – G. Charlot & D. Bezier (translated by R. C. Murray)
Quantitative Chemical Analysis – I. M. Kolthoff, E. B. Sandel, J. Meehan & S. Bruckenstein

Course ID: CHEM-SI32, CHEM-SI33, CHEM-SI41, CHEM-SI42, CHEM-SI43

Chemical Application of Group Theory – F. A. Cotton
Molecular Symmetry and Group Theory – Robert L. Carter
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. Ballahausen
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. Keev
Ionic Crystal Lattice & Non-Stoichiometry – N. N. Greenwood
Solid State Chemistry – N. B. Hannay
Solid State Chemistry & Its Application – A. R. West

Thermal Methods of Analysis – W. W. Wendlandt
Symmetry in Molecules – J. M. Hollar
Orbital Interactions in Chemistry – T. A. Albright , J. K Burdt & M. H. Whangbo
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. Hegedus & 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
An Introduction to Bioinorganic Chemistry – R. J. P. Williams
Inorganic Chemistry of Biological Processes – M. N. Hughes
Bioinorganic Chemistry – E. I. Ochiai
Principles of Bioinorganic Chemistry- S. J. Lippard and J. M. Berg.
Comprehensive Coordination Chemistry – G. Wilkinson, R. D.
Gillard & E. W. Abel (Eds.)
Bioinorganic Chemistry – R. W. Hay
Inorganic Aspects of Biological and Organic Chemistry – R. P. Hanzlik
General Principles of Biochemistry of the elements – E. I. Ochiai
Introduction to Bioinorganic Chemistry – D. R. Williams
Comprehensive Organometallic Chemistry – G. Wilkinson, F. G. A.
Stone & E. W. Abel (Eds.)
Organo Transition metal Chemistry – S. G. Davies
Nuclear and Radiochemistry – Friedlander, Kennedy & Miller
Essentials of Nuclear Chemistry – H. J. Armikar
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. Spenks & R. J. Woods
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
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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
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Crystal Structure Analysis for Chemists and Biologists, Jenny P. Glusker with Michell Lewis Miriam Rossi

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Quantitative Inorganic Analysis – A. I. Vogel
Quantitative Inorganic Analysis – G. Charlot & D. Bezier (translated by R. C. Murray)
Quantitative Chemical Analysis – I. M. Kolthoff, E. B. Sandel, J. Meehan & S. Bruckenstein
Instrumental Methods in Analysis – Willard, Merritt and Dean
Instrumental methods in Chemical Analysis – G. W. Ewing

Course ID: CHEM-SO32, CHEM-SO33, 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 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.
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Frontier Orbitals and Organic Chemical Reactions - I. Fleming.
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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.
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Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.
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Applications of Nuclear magnetic Resonance Spectroscopy in Organic Chemistry L. M. Jackman.
NMR in Chemistry - A Multinuclear A 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 - RO.C. Norman and J. M. Coxon-Blackie.
Some Modern methods, of Organic Synthesis - W. Carruthers.
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 Chemstry – Schneider, H.-J; Yatsimirski
Current Trends IN Organic Synthesis – Scolastico, C. & Nicotra, F.
Organic Synthesis - The Disconnection Approach - Stuart Warren
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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.
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Modern Methods in Carbohydrate Synthesis – Khan, S. H.; O'Neil, R. A.
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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.
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The Alkaloids - J.A. Cordell.
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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. Niclaou & 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 Encycloprdia 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

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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, Rodewaid & Wingrove.
Handbook of Organic Analysis - H.T. Clarke.
Systematic Qualitative Organic Analysis- H. Middleton.
Thin Layer Chromatography - Egon Stahl.
Spectrometric Identification of Organic Compounds – Silverstein & Webster; 6th edition

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Elementary Quantum Chemistry – F. L. Pilar
Quantum Chemistry – I. N. Levine
Modern Quantum Chemistry – A. Szabo, N. S. Ostlund
Molecular Quantum Mechanics – P. W. Atkins
Quantum Mechanics – J. L. Powell, B. Crasemann
Introduction to Quantum Mechanics – D. J. Griffiths
The Feynman Lectures in Physics, Vol. 3 – R. P. Feynman, R. B. Leighton, M. Sands
Chemical Applications of Group Theory – F. A. Cotton
Group Theory and Chemistry – D. M. Bishop
Coulson's Valence – R. McWeeny
Thermodynamics and an Introduction to Thermostatics – H. B. Callen
Elements 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,
Principles of Physical Biochemistry – K. E. van Holde, C. Johnson, P. S. Ho
Modern Electrochemistry – J. O'M. Bockris, A. K. N. Reddy
Physical Chemistry of Macromolecules – C. Tanford
Polymer Chemistry – P. J. Flory
Molecular Spectroscopy – I. N. Levine
Molecular Spectroscopy – J. D. Graybeal
Principles of Fluorescence Spectroscopy – J. R. Lakowicz
Introduction to Magnetic Resonance - A. Carrington, A. D. McLachlan
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 – A. J. Dekker
Molecular Modelling: Principles and Applications – A. R. Leach
Photodissociation Dynamics - R. Schinke
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
Microwave Spectroscopy – C. H. Townes and A.L. Schawlow
Laser Spectroscopy – W. Demtroder
Advanced Engineering Mathematics – E. Kreyszig
Mathematical Methods in the Physical Sciences – M. L. Boas

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Practical Physical Chemistry – A. M. James, F. F. Prichard
Findlay's Practical Physical Chemistry – B. P. Levitt
Experimental Physical Chemistry – Shoemaker and Garland
Computer Programming in Fortran IV – V. Rajaraman
Programming with Fortran – S. Lepschutz, A. Poe
Genetic Algorithm in Search Optimization and Machine Learning – D. E. Goldberg
Computational Intelligence – A. Konar
Numerical Recipes in Fortran – W. H. Press *et al*