UNIVERSITY OF CALCUTTA

NotificationNo.CSR/36/2022

It is notified for information of all concerned that the Syndicate in its meeting held on 24.11.2022 (vide Item No.24) approved & confirmed by the Syndicate the matter regarding the revised Syllabus of two years four semester M.Sc. course in Chemistry 2022, under this University, as laid down in the accompanying pamphlet.

The above shall be effective from the session 2022 -2023.

09/12/22

SENATE HOUSE
KOLKATA-700 073

Prof.(Dr.) Debasis Das
Registrar

REGISTRAR
UNIVERSITY OF CALCUTTA

SYLLABUS

FOR

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

CHEMISTRY

2022

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-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) **CREDIT POINTS** **CBCS** **CREDIT POINTS**	**150 100** **(12) (8)**	**150 100** **(12) (8)**	**50** **(4)** **100** **(8)**		**650** **(52)**
SPECIAL (S) **CREDIT POINTS**			**100** **(8)**	**150 100** **(12) (8)**	**350** **(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 Chemistry Special (SA)

(ii) Inorganic Chemistry Special (SI)

(iii) Organic Chemistry Special (SO)

(iv) Physical Chemistry 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	Pract	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	Pract	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	Pract	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

*One special course to be opted and continued systematically.
**Project or Practical (Students' Choice).

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 C. U.;

use of projector is mandatory ; time 10 min, followed by discussion.

Course ID:

CHEM–SA44/SI44/SO441/SP44

Project:

Continuous assessment	Project	Grand Viva
40 marks	40 marks	20 marks

Continuous assessment to be assessed by the guide;
Project to be assessed by External Expert;
Grand Viva to be taken by Sectional Faculty members and assessed by them.

OR

Practical:

Continuous assessment	Experiment	Grand Viva
20 marks	60 marks	20 marks

Continuous assessment to be assessed by the Sectional Faculty members conducting practical classes;
Exam on Experiments to be taken by the Sectional Faculty members conducting practical classes and assessed by them;
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. Magnetic properties – elementary idea.

Unit–3: EPR and Mössbauer Spectroscopy

Principle of EPR and 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 radicals and inorganic molecules (only one unpair electron systems) 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 Mössbauer active nuclei (iron) in variety of environments.

Unit–4: Bioinorganic Chemistry–I

Bioenergetic principle and role of ATP. Metal ion transport and storage proteins: ferritin, transferrin, ceruloplasmin. Electron transport proteins: cytochromes, Fe-S proteins, blue copper proteins and other electron carrier proteins in biology. Cobalamins including vitamin and coenzyme B12. Dioxygen storage/transport proteins: Hemoglobin, myoglobin, Hemerythrin and Haemocyanin. 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 (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–I

Conformational analysis of cyclohexane, cyclohexene, decalin and their derivatives; perhydroanthracene, perhydrophenanthrene etc. Stereochemistry of nucleophilic addition reactions to carbonyl compounds: Felkin-Anh, Cieplak and Zimmerman-Traxler Models. Curtin-Hammett principle.

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, Dewer-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 and torquoselectivity in electrocyclic 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: Mass Spectroscopy

Principles, instrumentation and applications of mass spectrometry. Methods of generation of ions in EI, CI, FD and FAB, ESI and MALDI.. 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.

COURSE ID: CHEM–G13

Unit–1: Interfacial Chemistry

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

Unit–2: Atomic Structure

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

Unit–3: Quantum Mechanics–I

Key features of quantum mechanics, Matter wave, de Broglie wave and Galilean transformation, Born interpretation of probability wave, wave packet,time evolution of wave function and time dependence of expectation values of Hermitian operators, Quantum-Classical correspondence, Stationary states under special potentials (step, rectangular barrier /finite square well), bound states in slowly varying potential, Wentzel–Kramers–Brillouin (WKB) approximation.

Unit–4: Kinetics–I

Fast reactions, Oscillatory reactions, Autocatalysis. Electrode kinetics: Nernst, Butler-Volmer and Tafel equations, rudimentary knowledge of PES, catalysts.

Unit–5: Polymer Chemistry

Classification of polymers, Kinetics of polymerization, Free radical mechanism (chain reactions), 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–I

(i) Spectrophotometric, ion exchange and complexometric estimations.

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

(iii) Experiments (Kinetics, equilibrium, electrochemistry, spectroscopy).

SEMESTER – II

Course ID: CHEM–G21

Unit–1: Chemical Bonding

Theories of Chemical Bonding – Valence Bond Theory and Molecular Orbital Theory. Molecular Orbital description of varieties of dinuclear, trinuclear and oligonuclear molecules. Walsh diagram. Evidence of MO pictures from spectra. 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–I

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 (η1 & η3), -carbonyl and cyclopentadienyl complexes with typical examples. Structure and bonding of $[(PPh_3)_2Pt(C_2Ph_2)]$, $[Mo(porphyrin)(C_2H_2)]$, $[Ni(\eta3\text{-}C_3H_5)_2]$ and $[FeCp_2]$. Reactions of organometallic complexes: Substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Unit–4: Boron Chemistry and Solid State Chemistry

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.

Defects in solids, zero-, one-, two- and three-dimensional defects, stoichiometric and non-stoichiometric defects, thermodynamics of the formation of defects, determination of equilibrium concentration of Schottky and Frenkel defects, colour centres in ionic crystals.

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 chemistry. Rates of nuclear decay: growth of radioactive products in a decay chain. Detection and measurement of radiation.

Course ID: CHEM–G22

Unit–1: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, *Cis-trans* isomerisation, 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 – Preparation and Chemistry of organo boron 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, TMSCN, 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 sulphoxonium ylides, chiral sulphoxides, umpolung

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: Chemical Bonding – Physical Aspects

Born-Oppenheimer Approximation and Beyond, Concept of PES, Nonadiabatic processes, Jahn Teller theorem, vibronic coupling, conical intersection Quantum Mechanical Virial theorem and role of electronic kinetic energy and potential energy in formation of covalent bonding, one electron and many electron contributions to chemical bond. Hellmann-Feynman theorem, Electrostatic theorem and concept of chemical bonding

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. Construction of orbitals, Spin, Role of constant motion.

Unit–3: Group Theory–I

Reducible and irreducible representations, Classes and Characters, Great Orthogonality theorem and related theorem, Projection operators, Direct product representation, Commutation relations among Hamiltonian and symmetry operators, Simultaneous eigen-functions, Construction of SALC, Selection rules in spectroscopy, Study of normal modes, IR and Raman activity.

Unit–4: Quantum Mechanics–II

Sequential Stern-Gerlach experiment, Vector space and operators, Diagonalization and simultaneous diagonalization of Hermitian operators, Cayley-Hamilton theorem,Schwarz inequality, Generalized uncertainty principle, Mandelstam-Tamm uncertainty relation and its implication, Quantum harmonic oscillators, Solving Hermite differential equation, Algebraic solution for the ground and excited states of QHO.

Unit–5: Biophysical Chemistry

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

Course ID: CHEM–G24

Practical Chemistry–II

(i) Qualitative analysis of mixture of inorganic compounds.

(ii) Organic preparation–I.

(iii) 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. 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

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; 6^{th} 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 Thermostatics – 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
Plymer 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, NMR and NQR Spectroscopy of Inorganic Molecules

Applications of IR spectra in organometallic compounds. NMR spectroscopy of inorganic compounds: ^{1}H, ^{13}C NMR spectra of paramagnetic complexes, dipolar and contact shifts and calculation of magnetic moment in solution by Evans method. ^{10}B, ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{17}O, ^{31}P and ^{195}Pt NMR spectroscopy in typical inorganic compounds. 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: Natural Products

Alkaloids: Biosynthesis, chemical synthesis, structure elucidation and physiological properties of Morphine, Coniine, Papaverine and Atropine.

Terpenoids: Biosynthesis, chemical synthesis and physiological activity of representative examples of acyclic, monocyclic and bicyclic monoterpenoids. Structural types and general introduction of sesquiterpenoids, diterpenoids and triterpenoids.

Steriods: Structural featurs, chemistry and physiological activity of steroids.

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.

SPECIAL PRACTICAL

Course ID: CHEM–SA31

Practical Analytical Chemistry:

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

Course ID: CHEM–SI31

Practical Inorganic Chemistry:

1. **Quantitative estimation of alloys and ores using titrimetric and spectrophotometric methods:**

(a) Analysis of brass (Cu and Zn) by iodometry and complexometry.

(b) Analysis of Steel (Cr, Mn, Ni, Cu and P) by spectrophotometry (Cr, Mn), titrimetry (Cr, Mn, Cu), gravimetry (Ni), alkalimetry (P).

(c) Analysis of Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2) by gravimetry (SiO_2), complexometry (Al^{3+}), redox titration using Jones reductor (Fe^{3+} and Ti^{4+}), spectrophotometry (Fe^{3+} as Fe-SCN complex, Ti^{4+} as Ti^{4+} - H_2O_2 complex).

2. **Physicochemical experiments:**

Composition of 1:1 (e.g. Fe^{III}-Sulphosalicylic acid) and 1:3 (e.g. Fe^{II}-*o*-phenanthroline) complexes by Job's, slope ratio and mole ratio methods using UV-Vis spectrophotometer/colourimeter; Kinetic study of the reduction of $[Co^{III}(NH_3)_5N_3]Cl_2$ by Fe^{II} using UV-Vis spectrophotometer/colourimeter; Kinetic study of aquation of $H[Co^{III}(HDMG)_2Cl_2]$ using conductivity meter and thermostat; Determination of stability constants; Etc.

3. **Syntheses and crystallization of coordination compounds:**

Synthesis of $[VO(acac)_2]$, $[M(acac)_3]$ (M = Cr, Fe, Co), $H[Co(dmgH)_2Cl_2]$**,** $[Co(NH_3)_5N_3]Cl_2$, $[Co(NH_3)_5Cl]Cl_2$, $[Co(NH_3)_6]Cl_3$, $[Ni(en)_3]Cl_2$, [Zn(salicylaldiminato)], $[Ni(PPh_3)_2Cl_2]$, $[Cr(oxaleto)].3H_2O$, etc. Crystallization of synthesized complexes.

Course ID: CHEM–SO31

Practical Organic Chemistry:

1. Separation and identification of the components of a binary mixture (Classical Method): FM 50
2. Organic preparation–II: FM 50

Course ID: CHEM–SP31

1. Detail aspects of programming language (Fortran).
2. Antibiotic kinetics, Verification of Onsagar equation, Iodination of aniline colorimetrically/analytically.

CBCS PAPER

CBCS CHEM (50 marks, credit 04)

(10 marks, 10 lecture hours for each unit)

Unit–1: Environmental Chemistry

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–2: Organometallic Chemistry and Catalysis

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. π-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.

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

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

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

Basic Principles and Applications:

Optical spectroscopy for chemical analysis, Atomic Absorption Spectrometry,

Radiochemical Analysis, Electrochemical Analysis: Voltammetry, Thermogravimetric Analysis

SEMESTER – IV

Course ID: CHEM–SA41

Unit–1: Elements of Electronics and Instrumentation–I

Basic structure of Chemical instruments. Transducers. Passive components and their properties. Semiconductor Diodes and Transistors. Amplifier properties. Negative and positive feedback. Operational amplifiers. Oscillators. Power supplies.

Unit–2: Elements of Electronics and Instrumentation–II

Non-linear and digital circuits – basic binary, logic gate counters, Microprocessors. Application to specific chemical instruments.

Unit–3: 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–4: 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. Polymer solution thermodynamics. Conjugated polymers and their electrical and opto-electronic properties.

Unit–5: Advanced Techniques in Spectroscopy and Microscopy

Time-resolved Fluorescence spectroscopy : principles of instrumentation and data analysis. Single Molecule Fluorescence. Fluorescence Correlation Spectroscopy. Fluorescence Lifetime Imaging. Optical Tweezers.

Course ID: CHEM–SI41

Unit–1: Chemical Application of Group Theory

Introduction - Construction of character tables, reducible and irreducible representations, direct product.

Splitting of orbitals and free-ion terms in various environments. Correlation diagrams. Tanabe-Sugano and Orgel diagrams. Symmetries of the first excited states of normal modes and utilization of these symmetries in spectroscopy. d-d transitions – transition selection rules, vibronic coupling, polarization, spectral parameters. Utilization of group theory in hybridization and molecular orbital description.

Unit–2: Advanced Coordination Chemistry

Introduction – Bonding theories and nomenclature of coordination compounds.

Varieties of organic and inorganic ligands based on - number and types of donor atoms, acyclic/cyclic nature (macrocyclic ligands including crown ethers, cryptates and spherand), diamagnetic/paramagnetic property, redox noninnocent/innocent property, σ/π-donor/acceptor aspect, strong/weak field aspect, bridging/chelating/encapsulating aspect. Discrete and polymeric metal complexes derived from various types of ligands – synthesis/characterization/studies/applications. Chelate effect, macrocyclic effect, cryptate effect. Electronic and steric effects governing the stability and lability of coordination compounds. Shape/geometry of coordination compounds. Isomerism, isomorphism and polymorphism. Design of ligands & metal complexes to get targeted properties and structure-property correlations.

Unit–3: Solid State Chemistry

Band Theory (Kronig-Penney Model), Bloch Theorem, Band gap, Metal, Insulator, Semiconductors. Semiconductors (Intrinsic and extrinsic), Hopping, rectifiers and transistors. Free Electron Theory, Electronic specific heat, Electrical and Thermal Conductivity of metals, Wiedemann-Franz law, Hall Effect, Superconductivity, Basic concepts of BCS theory, Meissner effect.

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, 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. Isolation. Lanthanide and actinide contractions and their consequences, role of relativistic effect. Oxidation states, redox and complex chemistry (including organometallic chemistry), reactivity, magnetic and spectral behaviour. f-block systems as NMR shift reagents, MRI contrast agents and superconductors.

Course ID: CHEM–SO41

Unit–1: Stereochemistry–II

Advanced course involving conformation and reactivity- acyclic system, allylic 1,2- and allylic 1,3- strain, bicyclic systems, tricyclic systems.

Chiroptical properties of organic molecules, CD, ORD-principles and applications, haloketone rules, sector rules. Baldwin's Rules-applications, hydrolytic and dynamic kinetic resolution.

Unit–2: Asymmetric Synthesis

Enantio- and diastereoselective synthesis. Reactions of enolates (α-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 and thiepines.

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 and Negishi coupling. Ziegler Naata reaction, Olefin metathesis, Tebbe's reagent, Pauson-Khand reactions, Vollhardt co-trimerisation, functional organometallic compounds. Use of nontransition metal Indium, tin, zinc.

Unit–5: Medicinal Chemistry–I

Synthesis, semi-synthesis, detailed mechanism of action and structural modifications of Penicillin antibiotics. General structure and antimicrobial activites of Cephalosporins, Tetracyclins and newer generation of antibiotics. General introduction on virus and mechanism of action of antiviral drugs towards DNA and RNA virus. General principle of vaccination strategy to combat with viral infection. Synthesis and mechanism of action of representative examples of antitumor, anticancer, antisense and DNA cleaving agents.

COURSE ID: CHEM-SP41

Unit–1: Quantum Mechanics–III

Tensor product space, Quantum Entangled states , Bell basis states, EPR and Bell inequality,Introduction to quantum computing, Position and momentum space representation, Delta function and Fourier transform, Pictures of quantum mechanics-

Schrodinger-Heisenberg-Dirac, Coherent state in Heisenberg picture, Spin precession in Dirac picture

Unit–2: Quantum Mechanics–IV

Time dependent perturbation from Dirac picture, Dyson series up to second order correction, Constant vs. Harmonic perturbation, Adiabatic and Sudden approximation, Rabi oscillation with example(ammonia atomic clock), Fermi-Golden rule, Atom-Light interaction.

Unit–3: Perturbation Theory

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

Unit–4: Quantum Chemistry–I

Basis and Applicability of Variation Method, linear variation method – secular determinant.

Many electron systems: Antisymmetrizer operator and determinantal wavefunction, self-consistent fields : Hartree and Hartree-Fock (HF) theories, Closed Shells : HF method, Koopmans' theorem, implementation of HF method – Roothaan equation, Open Shells : Restricted HF treatment and problems with it, Unrestricted HF.

Multiconfigurational wavefunctions, the structure of the full configuration interaction(CI) matrix – concept and consequence of Brillouin theorem

Unit–5: Quantum Chemistry–II

Concepts of static and dynamic correlation energy, intermediate normalization and expression of correlation energy,multiconfiguration self-consistent field (MCSCF) and the generalized valence bond (GVB) methods – elementary exposure, truncated CI and size-consistency problem, many-body perturbation theory,Fundamentals of Coupled cluster theory

Concepts in Density Functional Theory (DFT): Density, density matrices and functional, Hohenberg-Kohn theorem – concept and consequence, N- and v- representabilities,Kohn-Sham equation for the ground state of many electronic system – idea and implementation, Exchange Correlation functional and related concepts. Approximations in DFT: Local Density Approximation – Basics, merit and limitation.

Course ID: CHEM-SA42

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: 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: Forensic Analysis Methods

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−5: Environmental Chemistry of Atmosphere, Hydrosphere & Lithosphere

Characteristics of the atmosphere. Atmospheric stability and meteorology. Photochemical smog and Acid rain. Particles in the troposphere. Air pollutants – their source and effect, abatement and control. Antarctic Ozone Hole and Chlorofluorocarbons.

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.

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: Magnetochemistry

Definition of magnetic properties, types of magnetic bodies, experimental 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 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, 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 (preliminary idea), magnetic exchange interactions, Heisenberg-Dirac-van Vleck equation and its applications, Bleaney Bowers equation, magnetic materials.

Unit–2: Crystallography

Crystal and lattice, process of crystallizations, crystal form, habit, defect, lattice planes, indices, crystal systemsand symmetry, primitive and nonpremitive 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,lunes,crystal mosaicity and beam divergence, completeness ofdata 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 substation reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes; Solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation; Mechanism of isomerization reaction----linkage isomerism, cis-trans isomerisms, intermolecular and intramolecular recimization; 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

Basic concept and principles; the meaning of supramolecular chemistry, history, molecular recognition and hydrogen bonding; Secondary Electrostatic Interactions in Hydrogen Bonding Arrays. Different non-covalent interactions, Metal directed self-assembly, design of supramolecular host molecules. Examples of Host-guest complexes. Catalytic applications of molecular hosts. Metal Organic Frameworks (MOFs) and their applications, covalent organic frameworks.

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 ^{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, MRI as a diagonistic tool.

Unit–2: Bioorganic Chemistry

Molecular models of biological receptors, biomimetic chemistry, design, synthesis and binding studies of synthetic receptors. Proteins, peptides: solid-phase synthesis, and primary structure determination. Enzyme models, micelles, polymers, cyclodextrins, remote functionalization reactions, catalytic antibodies, Nucleic acids: Structure, sequence and synthetic principles. Principle of gene synthesis.

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, 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: 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–II

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, NOE, NOESY, COSY

Unit–3: Statistical Mechanics–I

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

Unit–4: Statistical Mechanics–II

Formulation of quantum statistical mechanics : pure and mixed states, density matrix, quantum Liouville theorem and its consequence, quantum statistics and ensembles. Specific heat of electron gas, Debye theory of specific heat of solids, Bose-Einstein condensate, Superonductivity, BCS theory

Unit–5: Mathematical Concepts

Extremum principle, Constrained extremization, Power series: Convergence and divergence, Taylor series and Fourier Series, Matrices – finding eigenvectors and eigenvalues and applications, Introduction to AI based techniques.

Course ID: CHEM–SA43

Unit–1: 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−2: 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−3: Thermal Analysis

Principle and Instrumentation of Thermogravimetric analysis (TGA), Differential thermogravimetric analysis (DTG), Differential thermal analysis (DTA), Differential Scanning Calorimetry (DSC) and other Thermal Analysis Techniques. A brief outline and a comparative discussion of DSC with DTA. Factors affecting the Thermal Analysis Curves. Applications of different thermal methods of analysis. Understanding of evaporation, sublimation, desolvation, decomposition, oxidation, reduction, glass transition and phase transition.

Unit−4: Bioanalytical Chemistry

Spectroscopic Methods for the Quantitation of Classes of Biomolecules-total protein, total nucleic acids, total carbohydrates and free fatty acids. Enzymes in Bioanalytical Chemistry, Experimental Determination of Michaelis-Menten Parameters, Quantitative Immunoassays with Labels-radioisotopes, fluorophores, Quantum Dots. Classification of Biosensors, DNA microarrays, Electrophoresis.

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 of the systems having more than one unpaired electron. Advanced Mössbauer spectroscopy of Sn compounds and multinuclear metal complexes or clusters of iron. Charge transfer spectra of coordination compounds.

Unit–2: Bioinorganic Chemistry–II

Dinitrogen fixation. Protective metalloenzymes such as superoxide dismutase, catalase, peroxidase. Metalloproteins catalyzing oxygen atom transfer reaction: cytochrome P-450, methane monoxygenase, 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. Metal ions in medicine including chelation therapy.

Unit–3: Organometallic Chemistry–II

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: Sensing of Analytes

Introduction - Jablonski diagram, photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, substitution, fragmentation, isomerisation, exchange and redox reactions, chemiluminescence, photochromism, determination of quantum yield.

Sensing of biologically relevant cations, anions and neutral molecules, chemosensors and chemodosimeters – fluorogenic and chromogenic. Mechanisms of sensing – PET, CHEF, ICT, ESIPT, FRET, C=N isomerization, AIE.

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 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 and Supramolecular Chemistry

Green catalysts and reagents: design, synthesis and applications in organic synthesis, nanocatalysts, surface modified catalysts, porous catalysts. Multicomponent reactions

(MCRs) for heterocycles synthesis under green conditions: mechanochemistry (Ball-Milling), reactions in micellar media, reactions in aqueous medium, reactions under solvent-free conditions.

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: Medicinal Chemistry–III

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.

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, Bloch theorem

Unit–2: Group Theory–II

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, Conservation of orbital symmetry, Understanding pericyclic reactions through Dewar-Zimmermann method (aromaticity of TS), Tanabe-Sugano diagram

Unit–3: Quantum Mechanics–V

Symmetries in quantum mechanics, Angular momentum as constant of motion, vector operators, Physical interpretation,Algebraic approach for the quantization of square of the generalized angular momentum operator and its z-component, Simultaneous eigenfunctions of L^2 and L_z operator, Matrix representations of angular momentum operators, Spin ½ and Pauli matrices, addition of angular momentum, (case study with l =1, s =1/2), Clebsch-Gordan coefficient.

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, CO_2, 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, Fermi resonance.

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Course ID: CHEM–SA44

(Students' choice - Project or Practical)

Project:

Internal assessment - 40 marks.

Presentation and project evaluation - 40 marks (by external examiner).

Grand viva - 20 marks.

OR

Practical Analytical Chemistry:

(Experiment 60 marks, internal assessment 20 marks, grand viva 20 marks):

1. Physico-chemical experiments based on instrumental techniques.

2. Computer-based experiments on statistical data analysis.

3. DFT calculations

(Some of the following instruments will be used while undertaking selected experiments: UV-Visible-NIR Absorption and FT-IR Spectrophotometers, Fluorimeter, NMR Spectrometer, Isothermal Titration Calorimeter, ESI-Mass Spectrometer).

Course ID: CHEM–SI44

(Students' choice - Project or Practical)

Project:

Internal assessment - 40 marks.

Presentation and project evaluation - 40 marks (by external examiner).

Grand viva - 20 marks.

OR

Practical Inorganic Chemistry

(Experiment 60 marks, internal assessment 20 marks, grand viva 20 marks):

1. Syntheses and studies of coordination and organometallic compounds under both aerobic and anaerobic conditions.
2. Ore/alloy analysis.
3. Physicochemical experiments.
4. Single crystal structure solution and refinement.
5. DFT calculations.

(Some of the following instruments will be used while undertaking selected experiments: UV-Vis, UV-Vis-NIR and FT-IR spectrophotometers; Fluorimeter; NMR Spectrometer; Single Crystal and Powder X-ray Diffractometers; ESI-MS; Isothermal Titration Calorimeter)

Course ID: CHEM–SO44

(Students' choice - Project or Practical)

Project:

Internal assessment - 40 marks.

Presentation and project evaluation - 40 marks (by external examiner).

Grand viva - 20 marks.

OR

Practical Organic Chemistry

(Experiment 60 marks, internal assessment 20 marks, grand viva 20 marks):

1. Chromatographic separation followed by spectroscopic characterisation - 20 marks
2. Organic preparation–III. - 40 marks
3. Grand Viva - 20 marks

Course ID: CHEM–SP44

(Students' choice - Project or Practical)

Project:

Internal assessment - 40 marks.

Presentation and project evaluation - 40 marks (by external examiner).

Grand viva - 20 marks.

OR

Practical Physical Chemistry

(Experiment 60 marks, internal assessment 20 marks, grand viva 20 marks):

A. Applications of numerical analysis in chemistry.

B. Advanced physico-chemical experiments.

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. 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
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 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
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Group Theory and chemistry – D. M. Bishop
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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
Symmetry in Molecules – J. M. Hollar
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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.
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Gordon Chemistry of Complex Equilibria – M. T. Beck & V.
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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
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
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Comprehensive Organometallic Chemistry – G. Wilkinson, F. G. A.
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Organo Transition metal Chemistry – S. G. Davies
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An Introduction to Inorganic Chemistry – K. F. Purcell & J. C. Kotz
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Orbital Symmetry - a Problem - solving approach.- R. E. Lehr and A. P. Marchand.
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Conservation of Orbital Symmetry – R. B. Woodward & R. Hoffman
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Frontier Orbitals and properties of Molecules - V. F. Tranen.
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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 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.
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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.

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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
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.
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Solvent-free Organic Synthesis – K. Tanka
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A Textbook of Practical Organic Chemistry - A.I. Vogel.
Qualitative Organic Analysis - A.I. Vogel.
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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 Thermostatics- 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. Steinfld, J. S. Francisco, W. L. Hase
Molecular reaction dynamics - R. D. Levine
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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

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Programming with Fortran – S. Lepschutz, A.Poe
Numerical Recipes in Fortran, The Art of Scientific Computing – W.H. Press, S.A. Teukolsky, W.T. Vellerling, B.P. Flannery