Structure and Detailed Syllabus of the
Postgraduate Course (M.Sc.) in Chemistry
Department of Chemistry
Presidency University
(Effective from Academic Year 2022-23)

PRESIDENCY UNIVERSITY
KOLKATA

Department of Chemistry

(Faculty of Natural and Mathematical Sciences)
Presidency University
Hindoo College (1817-1855), Presidency College (1855-2010)
86/1, College Street, Kolkata - 700 073
West Bengal, India

Aim of the Programme / Programme Outcomes:

1. Create an amicable learning environment among students to inculcate the deep interests and knowledge in subject.

2. Provide choice-based learning in specific sub discipline of chemistry.

3. Help students to develop the ability to use their knowledge and skills to interpret and handle the problem arises in day-to-day life.

4. Motivate students to pursue advanced studies on their subject of interest in the industry, academics and research institutions of repute.

5. Educate and enhancing student generic skills through skill enhancement courses, lab based, value added and project-based courses, this may help them creating employment and business opportunities in academia and industries.

Programme specific learning outcomes

A graduating student of M.Sc. Chemistry degree expected to:

1. Have proficient theoretical and experimental knowledge in the broad subject area of chemistry as well as different sub-fields of chemistry such as Analytical Chemistry, Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Material Chemistry, etc.
2. Explain, integrate and apply the acquired knowledge to problems that are emerging from the interdisciplinary areas.
3. Be aware of current developments at the forefront in Chemistry and allied subjects.
4. Have hands-on training on various analytical techniques, classical qualitative and quantitative chemical analysis, which enables their job opportunity on chemical industries and various nationalized analytical labs.
5. Have knowledge on hazardous chemical, safe handling of chemicals and role of chemistry on environmental issues.
6. Carry out experiments independently as well as be able to work productively in groups.
7. Construct a research problem as per the social requirement.
8. Communicate the scientific work in oral, written and e- formats as per the requirements.

Structure of Postgraduate Chemistry Course

Semester	Course Description with Marks						
	Theory						**Lab**
	Organic Chemistry	Inorganic Chemistry	Physical Chemistry	Common Paper	Special Paper (Organic/Inorganic /Physical)	Total	
First	50 (CHEM 0701)	50 (CHEM 0702)	50 (CHEM 0703)	-	-	150	Inorganic Lab: 50 (CHEM 0791) Physical Lab: 50 (CHEM 0792)
Second	50 (CHEM 0801)	50 (CHEM 0802)	50 (CHEM 0803)	-	-	150	Organic Lab: 50 (CHEM 0891) Computer Application: 50 (CHEM 0892)
Third	-	-	-	50 (CHEM 0901)	-	150	Advanced Organic /Inorganic/Physical Lab: 50 (CHEM 0991A/B/C) Research Based Lab: 50 (CHEM 0992)
				50 (CHEM 0902)	-		
	-	-	-	-	50 (CHEM 0903A/B/C)		
Fourth	-	-	-	-	50 (CHEM 1001A/B/C)	100	Project Work (CHEM 1091 and CHEM 1092): 50 + 50
					50 (CHEM 1002A/B/C)		
					50 (CHEM 1003) Seminar/Review and Grand Viva	50	
						600	**400**

Course Structure for two-year M.Sc. Programme in Chemistry (with effect from the academic session 2022-23) Semester-wise distribution of Courses

Semester	Paper Code	Name of the Courses	Full Marks	Credit Points	Course type†
1	**CHEM 0701**	General Organic Chemistry - I	50 (35 + 15)	4	T
	CHEM 0702	General Inorganic Chemistry – I	50 (35 + 15)	4	T
	CHEM 0703	General Physical Chemistry - I	50 (35 + 15)	4	T
	CHEM 0791	Inorganic Chemistry Lab	50	4	P, S
	CHEM 0792	Physical Chemistry Lab	50	4	P, S
		Total	**250**	**20**	
2	**CHEM 0801**	General Organic Chemistry - II	50 (35 + 15)	4	T
	CHEM 0802	General Inorganic Chemistry – II	50 (35 + 15)	4	T
	CHEM 0803	General Physical Chemistry - II	50 (35 + 15)	4	T
	CHEM 0891	Organic Chemistry Lab	50	4	P, S
	CHEM 0892	Computer Application	50	4	P, S
		Total	**250**	**20**	
3	**CHEM 0901**	Symmetry, Macromolecules and Magnetic Resonance	50 (35 + 15)	4	T
	CHEM 0902	Spectroscopy, Supramolecules and Nanomaterials	50 (35 + 15)	4	T
	CHEM 0903	Advanced Organic/Inorganic/Physical Chemistry -I *	50 (35 + 15)	4	T
	CHEM 0991	Advanced Organic/Inorganic/Physical Chemistry Lab**	50	4	P, S
	CHEM 0992	Research Based Lab	50	4	P, S
		Total	**250**	**20**	
4	**CHEM 1001**	Advanced Organic/Inorganic/Physical Chemistry -II*	50 (35 + 15)	4	T
	CHEM 1002	Advanced Organic/Inorganic/Physical Chemistry -III *	50 (35 + 15)	4	T
	CHEM 1003	Seminar/Review and Grand Viva	50	4	S
	CHEM 1091	Project Dissertation	50	4	P, S
	CHEM 1092	Project presentation, defense, proposal	50	4	P, S
		Total	**250**	**20**	
		Grand Total	**1000**	**80**	

† In Course Type, 'T' stands for Theory, P stands for Practical and 'S' stands for Sessional papers.

* Based on the specialization, Advanced Organic/Inorganic/Physical Chemistry theory papers, namely, CHEM0903, CHEM1001 and CHEM1002 are offered (semester 3 and 4) from respective sections: three streams differentiating A – Organic chemistry, B – Inorganic chemistry, and C – Physical chemistry.

** Based on the specialization, Advanced Organic/Inorganic/Physical Chemistry Lab paper (CHEM0991) is offered (semester 3) from respective sections: three streams differentiating A – Organic chemistry, B – Inorganic chemistry, and C – Physical chemistry

The methods of assessments for Sessional papers are continuous evaluation throughout the semester

The theory paper marks 50 (35+15) indicates (End semester examination 35 + Internal Assessment 15)

FIRST SEMESTER

Course No. CHEM 0701 (FM = 50; C = 4)
General Organic Chemistry-I

Course Objectives: This course aims to impart advanced level knowledge on (i) conformational aspects of alicyclic compounds and its implication in organic synthesis; (ii) the concept of concerted reaction, MO & symmetry of polyenes in controlling the stereochemical outcome of the reaction and its application in organic synthesis (iii) Modern spectroscopic techniques used in chemistry and the structure elucidation of organic compounds (problem solving) based on these techniques.

Unit 1: Stereochemistry (M = 15)

Static Aspects: Symmetry properties, point group; configuration – acyclic and cyclic systems; conformation – cyclic systems (cyclohexene, cyclohexanone, substituted cyclopentanes and cyclopentanones, medium rings, decalin and hydrindane systems).
Dynamic Aspects: cyclisation reactions, Baldwin's Rules; conformation and reactivity with reference to substitution, elimination, addition and rearrangement reactions.

Unit 2: Pericyclic reactions (M = 18)

Pericyclic reactions: Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – i) Frontier Molecular Orbital (FMO) approach ii) concept of aromaticity of transition states (Hückel / Möbius systems). The Woodward-Hoffmann selection rules and general rules.

General perturbation molecular orbital theory in cycloadditions: Symmetry principles in pericyclic reactions, orbital and state correlation diagram for electrocyclic and cycloaddition reactions. Reactivity, regioselectivity and periselectivity. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Ene reactions, group-transfer reactions and eliminations. Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems). Electrocyclic reactions of charged systems (cations and anions), Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

Sigmatropic rearrangements: [1, j] shifts – [1, 5] and [1, 7] shifts in neutral systems and [1,4] shift in charged species: [i, j] shifts – [3, 3] shifts, Sommelet-Hauser, Cope, aza-Cope rearrangements, Fluxional tautomerism. Claisen rearrangements; [5, 5] shifts, [2, 3] shifts in ylids.

Unit 3: Spectroscopy (M = 17)

Review of UV and IR spectroscopy ^{1}H NMR Spectroscopy: Basic theory – phenomenon of energy absorptions (resonance) and relaxation, chemical shift, shielding and deshielding mechanisms, equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry – Karplus equation. Structural application of ^{1}H NMR, aromaticity, antiaromaticity and homoaromaticity of organic molecules and related problems.

^{13}C NMR Spectroscopy: Principles; broad band decoupling, DEPT; structural applications of ^{13}C NMR.

Mass Spectrometry: Types of ionization techniques, basic principles of EI, fragmentation pattern of small molecules.

Problems incorporating spectroscopic data.

References:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen, Wiley India Ed, 2008.

2. Stereochemistry of Organic Compounds: Principles and Applications – D. Nassipuri, New Age International, 1994.

3. Advanced Organic Chemistry (Part A & B) - F.A. Carey and R. J. Sundberg,

Springer Science + Business Media, 5th Ed, 2007.
4. Organic Chemistry - J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2nd Ed, 2012.
5. The Conservation of Orbital Symmetry - R.B. Woodward and R. Hoffmann, Academic Press, 1971
6. Organic Reactions and Orbital Symmetry - P. L. Gilchrist and R. C. Storr, Cambridge [Eng.] University Press, 1972.
7. Pericyclic Chemistry -Orbital Mechanisms and Stereochemistry -D. K. Mandal, Elsevier, 2018.
8. Pericyclic Reaction - I. Fleming, Oxford University Press, 1998.
9. Molecular Orbitals and Organic Chemical Reactions - I. Fleming, John Wiley and Sons, Ltd.
10. Orbital Symmetry- A Problem-Solving Approach – R. E. Lehr, Alan P. Marchand, Academic Press INC, 1972.
11. Pericyclic Reactions - A Text Book: Reactions, Applications and Theory – S. Sankararaman, Wiley-VCH, 2005
12. Organic Spectroscopy - W. Kemp, ELBS
13. Introduction to Spectroscopy - D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Cengage Learning India Pvt. Ltd.
14. Applications of Absorption Spectroscopy of Organic Compounds – J. R. Dyer, Prentice Hall India Learning Pvt. Ltd.
15. Spectrometric Identification of Organic Compounds by R. M. Silverstein and G. C. Bassler, and T. C. Morrill, Spectrometric identification of Organic compounds, John Wiley & Sons, 5th Ed, 1991
16. Spectrometric method in Organic Chemistry - D.H. Williams and I. Fleming, Tata McGraw Hill Education.
17. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Günther, Wiley
18. Organic Structure Determination – J. H. Simpson, Elsevier
19. NMR Spectroscopy Explained – N. E Jacobsen, Wiley

Course Learning Outcomes: After completion of the course, the student should be able to

(i) Improve the basic idea of stereochemistry of organic compounds (small to large ring systems)

(ii) Analyze pericyclic reactions: Electrocyclic reactions, Sigmatropic Rearrangements and Cycloadditions and explain their feasibility in the light of

FMO approach.

(iii) Explain theoretical idea of nuclear magnetic spectroscopy (NMR), IR spectroscopy and Mass spectrometry to understand the spectra and characterize simple/complex organic molecules.

Course CHEM 0702 (FM = 50; C = 4)

General Inorganic Chemistry-I

Course Objectives: This course is designed to convey knowledge on basic and advanced level chemistry of coordination compounds, f-block compounds and Chemical equilibrium of inorganic complexes. Some special structural features of boranes and their industrial applications.

Unit 1 Coordination chemistry(I): Structure, stability and reactivity (M= 18)

Thermodynamic aspects of crystal field splitting, kinetics aspects of crystal field splitting, crystal field activation energy, labile and inert complexes. Single ion magnetic behavior, metal centered transitions.

Limitations of CFT, evidences of metal-ligand orbital overlap, nephelauxetic series; spectrochemical series. Free ion terms arising from d^n configuration and their splitting in Oh and Td fields – Orgel diagrams. Charge transfer spectra – LMCT and MLCT transition in Oh and Td complexes.

Structural and stereoisomerism of coordination compounds, optically active coordination compounds and their resolution procedures, absolute configuration of enantiomers.

Unit 2 Chemistry of elements: Special features (M = 16)

Structure and bonding of higher boranes, carboranes, metallocarboranes, Lipscomb's tropological diagrams and Wade's rules. Metal Clusters (low and high nuclearity carbonyl clusters), Skeletal electron counting, Wade-Mingos rule, application of iso electronic and isolobal relationships and caping rules. Metal-metal bonded complexes of metals (structure and bonding): dirhenium complexes, transition metal dioxygen and dinitrogen complexes (structure, bonding and reactivity), Vaska's complex. Alkali metal complexes with macrocyclic ligands, crown ether and cryptate complexes.

Unit 3 Chemistry of f-block elements (M = 8)

Relativistic effect; Magnetic properties and electronic spectra of lanthanides and actinides; use of lanthanide compounds as NMR-shift reagent and MRI-contrast agent; Super heavy elements

Unit 4 Chemistry of Complex Equilibria (M = 8)

Kinetic-, thermodynamic stability of metal complexes. Statistical and non-statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes. Determination of composition and stability constants of complexes by pH metric, spectrophotometric and polarographic methods. Solubility Equilibria – quantitativeness of precipitation (of metal hydroxides, sulphides and chelates).

References:

1. The f Elements - Nikolas Kaltsoyannis and Peter Scott
2. Concepts and Models of Inorganic Chemistry - Douglas, B.E. and McDaniel, D.H.
3. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed. - Huheey, J. E.; Keiter, E.A. & Keiter, R.L.
4. B.N. Figgies: Ligand Field Theory and its Applications General and Inorganic Chemistry: R. P. Sarkar, Vol II
5. Inorganic chemistry - Keith F. Purcell, John C. Kotz.
6. Multiple Bonds between Metal Atoms - Carlos A. Murillo, F. Albert Cotton, Richard A Walton, Richard A. Walton.
7. Inorganic Chemistry - Duward Shriver, Mark Weller, Tina Overton, Jonathan Rourke, Fraser Armstrong
8. Selected Topics in Inorganic Chemistry - W. U. Malik, G. D. Tuli, R. D. Madan.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Explain the origin of color using various theoretical phenomenon such as Orgel and Tanabe-Sugano diagram.
2. Explain the color intensity, reason of different color, reason of existence of

magnetism etc.

3. Explain lanthanide-based NMR-shift and MRI contrast reagent.
4. Determine the chemical composition and ligand lability properties using different techniques.
5. Structure and bonding of boranes using Lipscomb topological approach, Wade's rule and isolobal analogy.

Course No. CHEM 0703 (FM = 50; C = 4)
General Physical Chemistry-I

Course Objectives: To provide basic knowledge of molecular spectroscopy, partition function, ionic atmosphere and collision theory.

Unit 1 Molecular Spectroscopy (M=14)

Molecular spectroscopy: Introduction, elementary idea about spectroscopic instrumentation, spectral broadening. Electromagnetic spectrum and molecular processes associated with the regions. Rotational spectra of polyatomic molecules: classification of molecules into spherical, symmetric and asymmetric tops; linear triatomic molecules, Non-rigid rotor. Elementary idea of Stark effect. Anharmonic oscillator and dissociation. Elementary idea of Born-Oppenheimer approximation. Vibration rotation spectra for diatomic molecule, Rotational-vibrational coupling. Raman spectra: classical theory of Raman scattering, concept of polarizability ellipsoid.

Unit 2 Statistical mechanics- l (M = 12)

Probability, thermodynamic probability and entropy, Maxwell-Boltzman statistics, Partition function: translational (for ideal gas - concept of thermal wavelength), rotational, vibrational and electronic partition functions (diatomic molecule); molecular and molar partition function, Qualitative idea of Quantum statistics (Bose-Einstein, Fermi-Dirac statistics): Thermodynamic probability and distribution formula (without derivation), comparison with classical statistics - distinguishability and indistinguishability of identical particles.

Application: Theory of specific heat of solids – Einstein's and Debye's pictures.

Unit 3 Electrochemistry (M = 09)

Debye-Hückel theory of strong electrolytes, concept of ionic atmosphere. Debye-Hückel limiting law for single ionic activity coefficient and mean activity coefficient (with derivation), its relation to ionic strength. Bjerrum model for ion association: Formation of ion pairs, derivation of ion- association constant.

Unit 4 Kinetics-l (M = 15)

Collision theory: Lines of centre model. Introduction of potential energy surface and contour, internal coordinates and reaction coordinates, reaction path – valley and saddle point; saddle point – activation energy, classical trajectory, and theory of absolute rate. Comparison of collision and absolute rate theory. Fast reaction - relaxation methods. Branching chain reactions and explosion. Oscillatory reactions: Lotka-Volterra model and its applications.

Rate equation for electrode process. Butler-Volmer equation, High Field approximation, Tafel equation, Low field approximation, kinetic derivation of Nernst equation, exchange current density and polarizability of interfaces, concept of overvoltage. Kinetics of adsorption on solid, the adsorption isotherms (Langmuir, BET – with derivation)

References

1. Introduction to Atomic Spectra - White Harvey Elliott
2. Fundamentals of Molecular Spectroscopy - Banwell, C. N. & McCash, E. M.
3. Atomic Physics - Rajam J. B.
4. Introduction to Molecular Spectroscopy - Gordon M. Barrow
5. An Introduction to Statistical Thermodynamics - T. L. Hill
6. Statistical Mechanics - D. A. McQuarrie
7. Modern Electrochemistry 1: Ionics - J.O.M. Bockris; A.K.N. Reddy
8. An Introduction to Electrochemistry - S. Glasstone
9. Textbook of Physical Chemistry - S. Glasstone
10. Chemical Kinetics - Keith J. Laidler
11. Physical Chemistry - K.L. Kapoor
12. Physical Chemistry - Ashish K. Nag
13. Physical Chemistry - Gilbert W. Castellan

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain the fundamentals of rotational, vibrational spectroscopy, introduction of anharmonicity, basics of spectroscopic instrumentation of and spectra for polyatomic molecules and concept of polarizability in Raman scattering.
2. Explain the concept of thermodynamic probability, its relation with absolute entropy and express different thermodynamic energy parameters in terms of partition functions and Einstein's and Debye's pictures for specific heat of solids.
3. Describe the activity coefficients of electrolyte solution as a function of concentration.
4. Evaluate the ion-association constants of in solutions of weak electrolytes, and estimate the extent of associated ions.
5. Explain the difference between collision and absolute rate theory, kinetics of branching reaction, charge transfer process for electrode reaction and multilayer adsorption phenomena.

Course No. CHEM 0791 (FM = 50; C =4)
Inorganic Chemistry Lab

Course Objectives: The course aims to provide practical skill on estimation of inorganic ions using colorimetry, physiochemical methods and Quantitative estimation of ions in real life sample like milk and cola etc.

PART 1

Quantitative estimation of inorganic ions by colorimetry (any one).

Colorimetric determination of 1) Fe^{3+} as sulphosalicylate complex 2) Fe^{2+} as phenanthroline complex 3)Manganese as MnO_4^- 4) Chromium as dichromate.

Physicochemical Experiments:

i) Determination of composition of complexes by continuous variation/ Mole- Ratio / Slope ratio method of the following systems: Fe (III) – sulphosalicylate complex; Fe (II) - phenanthroline complex

ii) A colorimetric study of the kinetics on inorganic reaction.

Part II (any two)

1. Determination of the amount of calcium in milk powder by EDTA complexometry
2. Potassium trioxaltoferrate III: Sythesis, analysis and photochemistry.
3. Analysis of kidney stones by permanganometric titration
4. Preparation of $[Ni(NH_3)6]^{2+}$ and its analysis by different methods
5. Estimation of iodine in iodized common salt using iodometry
6. Estimation of phosphoric acid in cola drinks by molybdenum blue method
7. Paper and column chromatography of plant pigments

References:

1. A. J. Elias, A Collection of Interesting General Chemistry Experiments, Sangam books
2. G. N. Mukherjee, Advanced Experiments in Inorganic Chemistry, U. N. Dhur & Sons(p) ltd.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Estimate the various ions practically using colorimetric technique.
2. Estimate the various ions such as calcium, magnesium, phosphates, etc., present in real life day to day samples

Course No. CHEM 0792 (FM = 50; C = 4)
Physical Chemistry Lab

Course Objectives: To provide hand-on experiences of techniques for verifying physical and chemical properties and data interpretation skill.

1. Spectrophotometric experiment - determination of composition of a complex (Job's method)
2. Spectrophotometric experiment - Determination isosbestic point and indicator constant
3. Determination of cmc of surfactants: conductometry.
4. Determination of standard reduction potential of quinhydrone electrode.
5. Potentiometric determination of strength of halide mixture.
6. Determination of hydrolysis constant of NH_4Cl

7. Determination of molecular weight of macromolecules by viscometry.

Course learning outcomes: The students will acquire skills to

1. Handle instruments such as conductometer, potentiometer, spectrophotometer, viscometer, pH meter etc.
2. Analyze the data obtained from the experiments to measure various physico-chemical properties.

SECOND SEMESTER
Course No. CHEM 0801 (FM = 50; C = 4)
General Organic Chemistry-II

Course Objectives: This course aims to impart advanced level knowledge on (i) application of modern B, S, P and Si-based reagents in multistep organic synthesis (ii) designing synthetic strategies towards complex molecular targets such as bioactive heterocyclics and natural products including alkaloids, terpenoids and their structure elucidation.

Unit 1: Synthetic methodology and Synthetic strategy (M = 17)

Synthetic methodology: The roles of boron, phosphorus, sulfur and silicon in organic synthesis. Stereoselective hydroboration, hydrogenation, epoxidation and hydroxylation. Application of modern reagents in organic synthesis.

Synthetic strategy: Retrosynthetic analysis, disconnection, typical examples to illustrate the disconnection approach to organic synthesis.

Unit 2: Heterocyclic Chemistry (M = 17)

Systematic nomenclature (Hantzsch – Widman system) for monocycle and fused heterocycles.

General approach to heterocyclic synthesis – cyclisation and cycloaddition routes. Heterocycles in organic synthesis – masked functionalities, umpolung, Stork annulation reaction and applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc. Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

Unit 3: Natural products (M = 16)

Structural types; structure elucidation, reactions and synthesis of representative examples of (i) Alkaloids (ii) Terpenoids. Stereochemistry, reactions and synthesis of terpenoids and carotenoids: zingiberine, santonin, abietic acid, β-carotene. Stereochemistry, reactions and synthesis of alkaloids: quinine, morphine, camptothecin and recently discovered bioactive natural products.

References:

1. Modern Methods of Organic Synthesis - W. Carruthers, I. Coldham, CUP
2. Organic Chemistry - J. Clayden, N. Greeves, S. Warren and P. Wothers, OUP
3. Principle of Organic Synthesis - R.O.C. Norman and J.M. Coxon, Blackie

4. Organic Synthesis: The Disconnection Approach - S. Warren, Wiley
5. Organic Synthesis - M.B. Smith, McGraw - Hill
6. The Logic in Organic Synthesis - E.J. Corey and X. Cheng, Wiley
7. Organic Chemistry, Vol. II - I. L. Finar, ELBS
8. Mechanism and Theory in Organic Chemistry by Lowry and Richardson
9. Advanced Organic Chemistry: reactions, Mechanism and Structures (8th Edn) by J. March
10. Heterocycles in Organic Synthesis - A.I. Meyers, Wiley
11. Heterocyclic Chemistry - J.A. Joule and K. Mills, Blackwell
12. Heterocyclic Chemistry - T.L. Gilchrist, Wiley
13. Classics in Total Synthesis (Vol I) - K.C. Nicolaou and E.J. Sorensen, Wiley-VCH
14. Classics in Total Synthesis II - K.C. Nicolaou and S.A. Snyder Wiley-VCH

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explicate the use of modern reagent and their chemistry based on boron, silicon, sulphur, phosphorus and retro synthesis of complex molecule.
2. Expand the knowledge of simple and complex organic molecules containing one or more heteroatom.
3. Elucidate structures, stereochemistry, a variety of total synthetic pathways and reactions of classical and recently discovered bioactive natural products (alkaloids, terpenoids and carotenoids).

Course No. CHEM 0802 (FM = 50; C = 4)

General Inorganic Chemistry-II

Course Objectives: Impart knowledge on the VBT and LCAO-MOT theory on diatomic hydrogen type molecule and show orbital overlap in pictorial representation. Familiarize students with organometallic clusters, cages and their catalytic application. To provide an introduction into symmetry of molecules.

Unit 1 Aspects of Chemical Bonding (M = 16)

Born-Oppenheimer Approximation, Valence bond theory (VBT), resonance in VBT, VBT of homonuclear diatomic molecules. Hybridization, participation of d orbitals in hybridization in polyatomic species. Molecular orbital theory (MOT), linear combination of atomic orbitals (LCAO), criteria for the formation of stable

MOs. LCAO-MO Treatment of diatomic hydrogen (H_2) and hydrogen molecule ion (H_2^+). Sigma, Pi and Delta molecular orbitals. MO of Homonuclear and heteronuclear diatomic molecules and ions. MO theory of polyatomic molecules and ions. Walsh diagram. MO theory of conjugated molecules. Combination of atomic orbitals (pictorial approach). MO concept of metal-ligand bonding (pictorial approach)

Unit 2 Organometallic Chemistry (M = 17)

Preliminary idea and applications of 16 and 18 electrons rule for organometallic compounds. Reaction of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. Stereochemical non-rigidity and fluxional behaviour of organometallic compounds, catalysis by organometallic compounds: CH functionalization reactions. Applications of organometallics in organic synthesis: C-C coupling reactions (Kumada, Negishi, Heck, Suzuki, Hiama and Stille reactions etc).C-N bond coupling reactions and asymmetric hydrogenations. Polymerization, oligomerization and metathesis reactions of alkenes and alkynes; Zieglar-Natta catalysis.

Unit 3 Principle of symmetry in Chemistry (M = 17)

Concept of symmetry in molecules, symmetry elements and symmetry operations, combining symmetry operations. Multiplication Table by stereographic projection technique. Elements of Group Theory, Sub groups and classes of group elements. Symmetry point groups of molecules, systematic classification of molecular point groups, Application of symmetry in identifying polar and chiral molecules. Symmetry and stereo-isomerism. Unit vector transformation and interpretation of character table. Matrix representation of symmetry, matrix diagonalizations, Construction of character table, reducible and irreducible representations. Identification of symmetry label of MO in a molecule. Construction of MO on the basis of Symmetry of the molecules (H_2O, NH_3, B_2H_6, CH_4). Two-dimensional space group.

References

1. Fundamental Concepts of Inorganic Chemistry (Vol. 2), ed. 2 - A. K. Das.
2. General and Inorganic Chemistry (Vol. 1) - R. P. Sarkar.
3. A Textbook of Physical Chemistry (Vol. 4) - K. L. Kapoor.

4. Symmetry and Spectroscopy of Molecules - K. V. Reddy.
5. Chemical Applications of Group Theory - F. A. Cotton.
6. Group Theory in Chemistry - A. K. Mukherjee, B. C. Ghosh.
7. Basic Organometallic Chemistry - A. Elias, B. D. Gupta.
8. Principles of Organometallic Chemistry - Powell, P.
9. The Organometallic Chemistry of the Transition Metals - Crabtree, R. H.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Explain the concepts of VBT, and LCAO-MOT. The students should be able to represent orbital overlap diagram for sigma, pi- and delta bonding.
2. Explain the structures and electron counting schemes of organometallic compounds.
3. Demonstrate the structure and bonding, coordination modes, geometries, fundamental reaction types of organometallic compounds and the mechanisms in the organometallic catalytic processes.
4. Recognize symmetry elements in a molecule and deduce point group. Can represent matrices for symmetry representation.
5. Use character table to find out the symmetry labels for any orbitals and basis functions, which is extensively used in spectroscopy course. They will also be able to construct qualitative MOED diagram using character table.

Course No. CHEM 0803 (FM = 50; C = 4)
General Physical Chemistry-ll

Course Objectives: To impart basic knowledge of quantum mechanics, quantum numbers, atomic spectra and dielectric property.

Unit 1 Classical mechanics, limitations and prelude to new theories mechanics - l (M = 12)

Introductory ideas of classical mechanics – Equation of motion: Newtonian mechanics, Lagrangian mechanics, Hamiltonian mechanics, Classical mechanical Poisson bracket.
Failure of classical theories in back body radiation, specific heat of solid, photoelectric effects, and atomic spectroscopy; concept of quantization, identification of classical and quantum systems, Bohr's correspondence principle

with examples.
de Broglie relation, concept and properties of matter wave, comparison to travelling wave, dispersion relation, uncertainty principle, Plausible arguments leading to Schrödinger equation.

Unit 2 Quantum mechanics - l (M = 22)

Postulates of Quantum mechanics; state of the system; operators, Linear operators in quantum mechanics. Eigen value equation, Hermitian operator, measurement, probability concept, and continuity equation. Stationary state, elementary applications of time independent Schrödinger equation – different potential problems: free particle, confined particle in a box, step potential barrier problem: tunneling and its applications.
Heisenberg equation of motion, constant of motion, Ehrenfest's theorem. Commutator and relationship with Poisson bracket, non-compatibility and uncertainty; Formal derivation of Heisenberg uncertainty principle: commutability and compatibility.

Quantum mechanical treatment of simple harmonic oscillator; Rigid rotator; hydrogen atom.

Approximate method: Elementary perturbation theory, Variation theorem, Simple applications.

Unit 3 Atomic structure (M = 10)

Motion of angular momentum under magnetic field. Larmor precision. Stern Gerlach experiment. Spin-orbit interaction, conservation of total angular momentum J, Zeeman effect: Normal and Anomalous.

Motion under central force: Conservation of angular momentum and its consequence. Shape of different orbits, separation of radial and angular part. Shape of orbitals

Unit 4: Dielectric properties and inter-molecular forces (M = 6)

Dielectric polarization. Mossotti-Clausius relation, polar molecule. Debye equation. Dipole moment and molecular structure. Intermolecular forces. Attraction and repulsion potentials: van der Waals forces, Keesom, Debye and

London forces, their relative contribution; Lennard-Jones potential.

References

1. Quantum Mechanics - Cohen-Tannoudji, C.; Diu, B.; Lalöe, F.,. Wiley-Interscience: Paris, 1977;
2. Quantum Mechanics Concepts and Applications, Second Edition, - Nouredine Zettili.
3. Quantum Mechanics in Chemistry - Schatz, G. C.; Ratner, M. A
4. Quantum Chemistry, 7 th Edition - Ira N. Levine.
5. Introduction to Quantum Mechanics - David J. Griffiths.
6. Quantum Chemistry: An Introduction - Walter Kauzmann.
7. Theory of electric polarization - C.J.F. Bottcher.
8. Introduction to electrodynamics - David J. Griffiths.
9. Dielectric phenomena in solids - Kwan Chi Kao.
10. Classical Mechanics - H. Goldstein.

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain basic theory of classical mechanics with its failure to explain black body radiation, photoelectric effect, atomic spectra and concepts of matter waves with various arguments to reach Schrödinger equation.
2. Solve Schrodinger equation for various quantum chemical models such as, particle in a box, harmonic oscillator, rigid rotor models and H-atom,
3. Apply operator algebra to calculate eigen values and eigen functions of angular momentum
4. Apply various approximation methods to solve Schrodinger equation in presence of small perturbation and for multielectronic system.
5. Explain the idea of spin quantum number via Stern-Gerlach experiment, effect of magnetic field to atomic spectra and ideal of the shape of the orbits and orbitals.
6. explain the concept of dielectric polarization via deriving Mossotti-Clausius relation and possible intermolecular forces with their contribution.

Course No. CHEM 0891 (FM = 50; C = 4)
Organic Chemistry Lab

Course Objectives: To impart practical skill on Separation of binary organic mixtures

Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components by chemical and spectroscopic methods.

References:

1. Systematic Organic Qualitative Analysis – H. Middleton
2. Hand Book of Organic Analysis – H.T. Clarke
3. Qualitative Organic Analysis – A.I. Vogel

Course Learning Outcomes: After completion of the course, the student should be able to

1. Determine chemical composition from binary mixture of organic compounds.
2. Identify organic components by chemical and spectroscopic methods.

Course No. CHEM 0892 (FM = 50; C = 4)
Computer Application

Course Objectives: To provide basic understanding of the programming language, numerical methods, various computational techniques and to impart skills to apply them to solve problems related to chemistry.

Introduction to programming languages; basic numerical analysis: solution of nonlinear equations using Newton-Raphson method (e.g. finding the roots of a cubic equation – vander Waals equation), solution of linear systems using Gaussian elimination, interpolation, numerical integration (trapezoidal and Simpson's $1/3^{rd}$ rule), numerical solution of differential equations (Euler and Runge-Kutta method). Fourier transformations and applications in spectroscopy. Use of molecular geometry optimization software (Gaussian 09); construction of z-matrix and concept of force field.

Classical Molecular Dynamics (MD) simulation and application to simple systems like Lennard-Jones fluids.
[Effort should be made to reproduce data reported in the literature using the above-mentioned numerical methods wherever possible.]

Course learning outcomes: The students will explain and acquire skills to

1. Write computer programs to solve linear systems using Gaussian elimination, interpolation, numerical integration and numerical solution of differential equations.
2. Perform Fourier transformations and its applications in spectroscopy.
3. Use quantum chemical programs to do molecular geometry optimization and frequency calculation on chemically relevant systems
4. Perform classical Molecular Dynamics (MD) simulation on biologically relevant systems.

THIRD SEMESTER
Course No. CHEM 0901 (FM = 50; C = 4)
Symmetry, Macromolecules and Magnetic Resonance

Course Objectives: The objective of this course is to provide basic knowledge of character table, material chemistry and NMR, ESR.

Unit 1 Elementary Group Theory and Application of Symmetry (M = 20)

Introduction, symmetry elements and group theory, group theory and quantum mechanics (elementary ideas), elementary ideas of representation theory, irreducible representations of point group, definitions of classes and character, statement of grand orthogonality theorem, orthogonality theorem for characters, character tables, concept of character projection operator.
Selection rules in molecular spectroscopy, electronic spectroscopy and crystal field theory. SALC – Hückel, Hybridization. Vibration of polyatomic molecules
– normal modes, their symmetry properties and IR activity.

Unit 2 Polymer Chemistry (M = 08)

Classification of polymers, kinetics of two-dimensional polymerization, condensation and addition polymerizations; initiation, propagation and termination; chain transfer, co-polymerization; molecular weight of polymers; determination of molecular weights. Thermodynamics of polymer solution: entropy, heat and free-energy of mixing.

Unit 3 Colloids and Macromolecules (M = 07)

Introduction to nanomaterial, Lyophobic and lyophilic sols, origin of charge and stability of lyophobic colloids, coagulation and Schultz-Hardy rule, zeta potential and Stern double layer (qualitative idea); Tyndall effect, electrokinetic phenomenon (qualitative idea only); Microporous materials, microgels, bioconjugate polymers, gels, ointments and creams, biodegradable polymers. Fundamentals of nano science: definition, nano versus bulk, quantum confinement: nanoscale in 1D, 2D and 3D with examples, synthesis of nano materials: top-down and bottom-up approaches, size dependent properties; nanoclusters and nanowires, semiconductor nanoparticles, applications of nano materials.

Unit 4 Spin Magnetic Resonance Spectroscopy (M = 15)

Magnetic resonance spectroscopy – introduction, basis features of spectroscopy, relaxation processes: spin-spin and spin-lattice.

NMR: chemical shift and spin-spin coupling; chemical shielding – elementary idea of diamagnetic and paramagnetic shielding.

ESR: ESR spectrometer, line width, hyper-fine splitting, ESR of triplet state, applications.

References:

1. Group theory and chemistry - D. M. Bishop.
2. Group theory and Quantum chemistry - M. Tinkham
3. Fundamentals of Polymerization - Broja Mahan Mandal
4. Principles of Polymerization - George Odian
5. Physical Chemistry - Gilbert W. Castellan
6. Physical Chemistry - K.L. Kapoor
7. Principles of Physical Chemistry - Puri Sharma Pathania
8. Physical Chemistry - P.C. Rakshit
9. Physical Chemistry - H.C. Chatterjee
10. Introduction of nanomaterials - Asim Kumar Das

Course Learning Outcomes: After completion of the course, the student should be able to

1. Elucidate point group of various geometry, construct matrix representation for point groups, character table and apply the concept to spectroscopy, crystal field theory.
2. Derive the rate expression for polymerization process, ΔS, ΔG, relative vapor pressure and explain the properties of colloidal solution, concepts of nanoscience.
3. Explain theory and instrumentation of magnetic spectroscopy and its application for chemical analysis.

Course No. CHEM 0902 (FM = 50; C = 4)
Spectroscopy, Supramolecules and Nanomaterials

Course Objectives: To impart knowledge on theory of advanced spectroscopy, basic LASER principle, spectrometry and supramolecular Chemistry

Unit 1 FT NMR, FT IR, 2D NMR, Mass spectrometry (M = 18)

Fourier transformations, time domain versus frequency domain. Principles of FT NMR, instrumentation, the rotating frame of reference, simple 1D experiments. FT IR – principles and instrumentation.

Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE,

INDOR, INEPT for simple compounds and problems. Applications of multinuclear NMR in inorganic compounds – Examples from ^{1}H, ^{11}B, ^{13}C, ^{19}F, ^{31}P. NMR of paramagnetic molecules – Lanthanide shift.

Mass spectrometry: Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS and MS/MS techniques. Interpretation of spectroscopic (NMR, IR and mass) data, as applied to organic, inorganic and biological systems.

Unit 2 Electronic Spectroscopy (Absorption and Emission) (M = 15)

Einstein theory of Absorption and emission – A, B coefficients, Principles of LASER and characteristic features. Electric dipole transition – comparison of experimental and theoretical parameters, oscillator strength

Qualitative treatment of Born-Oppenheimer separation, Frank-Condon principle, Quantum mechanical interpretation of transition, selection rules, spin orbit coupling, vibronic coupling, characteristics of π-π^*, n-π^*, charge transfer transitions and their intensities.

Photoluminescence: fluorescence and phosphorescence, mirror-image symmetry, radiation less deactivation – internal conversion and inter system crossing. First order kinetics for excited molecule. Delayed fluorescence.

Quenching of fluorescence, Life-time variation in presence of quencher. Excimers and exciplexes. Intermolecular energy transfer. Excited state proton transfer. Modern experimental techniques in fluorescence spectroscopy.

Unit 3 Supramolecular Chemistry & Introduction to Nanomaterials (M = 09)

Introduction, Origins and Concept. Molecular recognition. Host-guest complex. supramolecular orbitals, non-covalent forces: soft interactions, Supramolecular reactivity and catalysis. Self-assembly and self-organization, Liquid crystals and supramolecular polymers, polymer-surfactant interaction. Molecular sensors and supramolecular devices.

Nanoparticles and nanomaterials, elementary idea of synthesis, nano-composites, applications (special attention in drug design). Microporous materials, microgels, bioconjugate polymers, Nanoencapsulation.

Unit 4 Mossbauer spectroscopy, PES, XPS and Applications (M = 08)

Principles of Mossbauer spectroscopy: experiments, center shift, quadrupole interaction, magnetic interaction. PES - photoexcitation and photoionization; XPS - principle and applications.

References:

1. Organic Spectroscopy - W. Kemp, ELBS
2. Introduction to Spectroscopy - Pavia, Lampman
3. Applications of Absorption Spectroscopy of Organic Compounds - Dyer
4. Spectrometric Identification of Organic Compounds - R. M. Silverstein and G. C. Bassler
5. Spectrometric method in Organic Chemistry - D.H. Williams and I. Fleming.
6. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Gunther, Wiley
7. Organic Structure Determination - Jeffrey H Simpson
8. NMR Spectroscopy Explained - Neil E Jacobsen
9. . Modern Molecular Photochemistry - Nicholas J. Turro
10. Principles of Fluorescence Spectroscopy, 3rd edition - Joseph R. Lakowicz.
11. Fundamentals of Photochemistry - K K. Rohotgi Mukherjee
12. Supramolecular Chemistry: Concepts and Perspectives - J. -M. Lehn

Course Learning Outcomes: After completion of the course, the student should be able to

1. Analyze the spectroscopic data, as applicable to organic, inorganic and

biological systems.
2. Analyze the possible photophysical processes for electronically excited molecules
3. Explain selection rule and their relaxation for electronic transition
4. Explore the use of supramolecular material chemistry in modern chemical society

Course No. CHEM 0903A (FM = 50; C = 4)
Advanced Organic Chemistry -I

Course Objectives: To impart advanced level knowledge on (i) stereochemical aspects of fused polycyclic systems including steroids and their application in synthesis (ii) molecular organic photochemistry including fundamental principles, primary photochemical reactions along with synthetic applications (iii) biogenesis of natural products and their role in metabolic pathways.

Unit 1: Stereochemistry of polycyclic system (M = 14)

Conformation and reactivity of fused polycyclic systems – perhydrophenanthrenes, perhydroanthracenes, steroids; Stereochemistry of reactions – nucleophilic additions to cyclic ketones, Cieplak model; directed nucleophilic additions.

Unit 2 Organic Photochemistry and Radical Reactions (M = 18)

Photochemistry: Photolysis of carbonyl compounds and nitrites: Norrish Type I and Type II processes, β-cleavage, Barton reaction. Photoreduction and Photoexcitation; Photorearrangements in cyclohexanones and cyclohexadienone systems; Photorearrangements of α-tropolone methyl ether, di-π-methane rearrangement (cyclic system) Photochemistry of organic compounds: photoisomerisation, phodimerisation, cycloadditions of benzene and its derivatives.

Radical Chemistry: Generation and detection of radicals, radical initiators, reactivity pattern of radicals, substitution, addition and cyclization reactions; Radical cations and radical anions, single electron transfer reactions.

Unit 3: Chemistry of Natural Products (Synthesis and Biosynthesis) (M = 18)

Introduction: Primary and secondary metabolites, biogenetic hypothesis, elucidation of biosynthetic pathways; Biosynthesis of terpenoids and steroids; Shikimic acid pathway: Biosynthesis of flavonoids; Biosynthesis of alkaloids; Synthesis and biosynthesis of polyketides, fatty acids and prostaglandins; Reactions and synthesis of steroids: cholesterol, bile acid, testosterone, estrone, progesterone; Structure and synthesis of porphyrins: haemoglobin, chlorophyll.

References:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.
2. Stereochemistry of Carbon Compounds - E.L. Eliel and S. H. Wilen.
3. Stereochemistry of Organic Compounds: Principles and Applications - D. Nasipuri.
4. Mechanism and Theory in Organic Chemistry - Lowry and Richardson.
5. Organic Photochemistry – J. M. Coxon and B. Halton.
6. Organic Chemistry, Vol. II - I. L. Finar.

Course Learning Outcomes: After completion of the course, the student should be able to

1. Demonstrate advanced idea of stereochemistry of fused polycyclic organic compounds.
2. Implement the basics of organic photochemistry and radical chemistry.
3. Interpret structures, laboratory and biosynthetic pathways for the generation of several primary, secondary metabolites and complex natural products.

Course No. CHEM 0903B (FM = 50; C = 4)

Advanced Inorganic Chemistry -I

Course Objectives: To provide the knowledge on applications of group theory, various aspects of magnetochemistry, solid-state chemistry

Unit 1 Chemical Application of Group Theory (M = 17)

Importance of group theory in inorganic chemistry, splitting of orbital and free ion terms in crystal fields, quantitative relationship between Oh & Td splittings, construction of energy level in infinitely strong crystal field, the effect of distortion on d-energy levels, vibronic coupling and vibronic polarization, utilization of symmetry and group theory in constructing the MO diagrams of polyatomic molecules, coordination complexes including metallocene complexes. Symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions.

Unit 2 Magnetochemistry (M = 18)

Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic system, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of *J* levels, 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, low spin, high-spin crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. Experimental arrangements for determination of magnetic susceptibility: SQUID. Preliminary idea about single molecular magnets.

Unit 3 Solid state chemistry and X-ray crystallography (M = 15)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors – intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism. Defects in solids.

The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering factor, structure factor, systematic absences, Determination of space groups and crystal structures.

References:

1. Chemical Applications of Group Theory - F. A. Cotton.
2. Magnetochemistry - A. Earnshaw.

3. Elements of Magnetochemistry - R. L. Dutta, A. Shyamal.
4. An Introduction to X-Ray Crystallography - M. M. Woolfson.
5. X-Ray Diffraction Methods - E. W. Nuffield.
6. X-ray Crystallography - M. J. Buerger.
7. Solid State Chemistry - D. K. Chakrabarty.
8. Crystallography Applied to Solid State Physics - A. R. Verma & O. N. Srivastava.
9. Structure of Metals - Charles Barret & T. B. Masalski.
10. Introduction to materials Science for Engineers - J. F. Shakelford & M.K. Muralidharan.
11. Superconductivity - R. G. Sharma.
12. Physical Chemistry - I. R. Levine.
13. Theoretical Chemistry - S. Glasstone

Course Learning Outcomes: On completion of the course, the students should be able to

1. Apply group theory to understand the vibrational spectroscopy of different complexes and CFT of coordination complexes.
2. Analyze the magnetic properties of different mononuclear and polynuclear metal complexes.
3. Measure the magnetic properties using SQUID.
4. Describe the origin of the conductivity in metallic conductors, semiconductors and superconductors.
5. Explain the molecular origin of dia-, para- and ferromagnetisms.
6. Quantify the extent of defects in solids.
7. Gain a comprehensive knowledge on the interaction between X-rays and crystalline solids and determine the space groups of crystals.

Course No. CHEM 0903C (FM = 50; C = 4)
Advanced Physical Chemistry -I

Course Objectives: To impart knowledge of various statistics, dielectric behavior, solvent effect on spectra, structures of solids and different rate processes.

Unit 1 Statistical mechanics- II (M = 15)

Concept of the macroscopic and the microscopic states, Statistical conditions for thermal, mechanical and chemical equilibrium; and connection between total micro-states and thermodynamics key quantities.

Concept of ensemble and ergodic hypothesis, phase space; microcanonical ensemble, counting micro-states, Gibbs paradox, correct enumeration of the microstates, Sackur-Tetrode equation;

Canonical ensemble distribution, probability distribution function, its relation with different thermodynamic state functions; application to a system of harmonic oscillators; the statistics of paramagnetism, energy fluctuations in the canonical ensemble, equipartition and the virial theorem. chemical potential and chemical equilibrium – Saha ionization formula;

Grand canonical ensemble – Density and energy fluctuations in the grand canonical ensemble: correspondence with other ensembles; phase equilibrium.

Nature of quantum particles; Bose-Einstein and Fermi-Dirac distributions; black body radiation and photon gas, Bose-Einstein condensation; Thermodynamic behavior of an ideal Fermi gas; the electron gas in metals.

Unit 2 Dielectric behaviour and solvent effect (M = 10)

Limitation of Mossotti-Clausius, Debye equation, deviation from Debye's theory; Onsager reaction field; dielectric relaxation, frequency dependent dielectric property, relaxation time, Debye semicircle; Solvent effect on the emission and absorption spectra - non- specific and specific interactions (H-bonding and charge transfer). Lippert equation; time resolved spectroscopy and the solvent relaxation.

Unit 3 Solid state chemistry and X-ray crystallography (M = 15)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors – intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism. Defects in solids.

The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering.factor, structure factor, systematic absences, Determination of space groups and crystal structures.

Unit 4 Kinetics - II (M = 10)

(a) Rate constant expression for chemical reaction based on Eyring equation with one example.

(b) Physical rate processes – viscosity and diffusion.

(c) Non- equilibrium formulation: Passage to statistical approach – energy redistribution in activated complex, Lindemann collision, Hinshelwood suggestion, Rice-Ramsperger-Kassel (RRK) theory.

(d) Reaction in solution. Diffusion-controlled reactions.

References

1. Statistical Mechanics – R. K. Pathria.
2. Introduction to Statistical Physics - Kerson Huang.
3. Fundamentals of statistical and thermal physics – F. Rief.
4. Statistical Mechanics - Donald A. McQuarrie.
5. An Introduction to Statistical Thermodynamics - Terrell L. Hill
6. Statistical Mechanics and Thermodynamics - Claude Garrod.
7. Heat and Thermodynamics – M. W. Zamansky, and R. H. Dittman.
8. Theory of electric polarization, - C. J. F. Bottcher.
9. Introduction to electrodynamics - David J. Griffiths
10. Dielectric phenomena in solids - Kwan Chi Kao.
11. An Introduction to X-Ray Crystallography - M. M. Woolfson.
12. X-Ray Diffraction Methods - E. W. Nuffield.
13. X-ray Crystallography - M. J. Buerger.
14. Solid State Chemistry - D. K. Chakrabarty.
15. Crystallography Applied to Solid State Physics - A. R. Verma and O. N. Srivastava.
16. Structure of Metals - Charles Barret and T. B. Masalski.
17. Introduction to materials Science for Engineers - J. F. Shakelford & M. K. Muralidharan.
18. Superconductivity by R. G. Sharma.
19. Physical Chemistry - I. R. Levine.
20. Theoretical Chemistry - S. Glasstone.
21. Chemical Kinetics - Keith J. Laidler.

22. The Theory of Rate Processes - Samuel Glasstone , Keith J. Laidler , Henry Eyring.
23. Dielectric Properties and Molecular Behaviour - Nora Hill
24. Principles of Fluorescence Spectroscopy - Joseph R. Lakowicz.

Course learning outcomes: After the completion of the course, the students should be able to

1. Describe the various ensembles equipartition theorem and its validity, Saha ionization formula, correlate Bose-Einstein and Fermi-Dirac statistics.
2. Express the limitation of Mossotti-Clausius equation, role of solvent to absorption- emission spectra and explain the time resolved emission spectra due to solvent relaxation.
3. Explain the molecular origin of dia-, para- and ferromagnetisms.
4. Quantify the extent of defects in solids.
5. Gain a comprehensive knowledge on the interaction between X-rays and crystalline solids and determine the space groups of crystals.
6. Apply Eyring equation, explain the behavior of diffusion-controlled reactions and Lindemann collision, RRK theory

Course No. CHEM 0991A (FM = 50; C = 4)
Advanced Organic Chemistry Lab

Course Objectives: To impart hands on training on multistep synthesis of organic compounds and their characterization

Multistep synthesis of organic compounds using typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PC, determination of R_f value as required, m.p/b.p.]. Characterization of organic compounds by spectroscopic means.
Extraction and Purification of Natural Products and Biomolecules.

References:

1. Systematic Organic Qualitative Analysis – H. Middleton
2. Hand Book of Organic Analysis – H.T. Clarke
3. Qualitative Organic Analysis – A.I. Vogel

Course Learning Outcomes: After completion of the course, the student should be able to

1. Deal with various synthetic problems
2. Handle sophisticated chemicals for synthetic application
3. Improve their analytical skills for separation and characterization.

Course No. CHEM 0991B (FM = 50; C=4)
Advanced Inorganic Chemistry Lab

Course Objectives: The course aims to provide practical knowledge on analysis of ores, minerals and alloys, synthesis and characterization of some interesting transition metal complexes.

1. Quantitative analysis of complex inorganic materials *viz.* ores, minerals and alloys etc. by conventional method. (any one)
2. Synthesis and characterization of Inorganic Compound
3. Preparation of transition metal complexes and their characterization

Course Learning Outcomes: On completion of the course, the students should be able to

1. Analyze the components of alloys, ores etc.
2. Able to handle the apparatus in synthetic lab
3. Able to interpret the characterization data

Course No. CHEM 0991C (FM = 50; C = 4)

Advanced Physical Chemistry Lab

Course Objectives: To provide hand-on experiences of techniques for verifying physical and chemical properties.

1. Tensiometry

2. Autocatalysis

3. Fluorescence quenching

4. Excited State Proton Transfer

5. Resonance Energy Transfer

6. Kinetic Salt effect

7. Onsager Theory (updated and modified version) – Conductance measurement

8. Solubility Product – Conductance measurement

9. Ternary Phase diagram

10. Clock reaction

Course learning outcomes: The students will acquire skills to

1. Evaluate rate constant, rate constant at zero ionic strength and Debye Hückel constant by spectrophotometry instrument for ionic reaction.
2. Elucidate individual order of the reactants for redox reaction by clock method.
3. Plot ternary phase diagram on two dimensions for water, chloroform, acetic acid system.

Course No. CHEM 0992 (FM = 50; C = 4)
Research Based Lab

Course Objectives: The course aims to provide advance practical/hands-on skills on the active research fields in departmental research laboratories to enhance their employability scope in academia and industry. Some of the active research areas are given below.

1. Synthetic organic chemistry
2. Synthetic inorganic and material chemistry.
3. Energy storage device
4. Polymer Chemistry
5. Computational Chemistry
6. Theoretical Chemistry
7. Spectroscopy
8. Environmental Chemistry

Course Learning Outcomes: On completion of the course, the students should be able to

1. Explore current research problems
2. Prepare themselves to handle research projects

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FOURTH SEMESTER
Course No. CHEM 1001A (FM = 50; C = 4)
Advanced Organic Chemistry -II

Course Objectives: This course aims to foster an understanding of (i) the key aspects of coordination compounds of transition metals along with a detailed knowledge of catalytic and industrial uses of organometallic compounds (ii) the importance of asymmetric synthesis, the concept, the biological relevance and a critical knowledge about the synthetic strategies available to us (iii) advanced level target-oriented synthesis of biologically relevant molecules employing various modern reagents.

Unit 1: Organotransition Metal Chemistry: Applications to Organic Synthesis (M = 17)

Electron counting, bonding, organometallic reaction mechanism; Homogeneous hydrogenation; Organometallics as electrophiles; Synthetic applications of transition metal alkene complexes: Wacker oxidation. Synthetic applications of complexes containing metal – carbon σ bonds: Heck and related reactions, carbonylation reactions; Synthetic applications of transition metal carbene complexes: Fischer carbene, Schrock carbene, metathesis processes, Tebbe's reagent, Zieglar – Natta reaction; Synthetic applications of transition metal alkyne complexes: Pauson – Khand reaction, cyclooligomerisation; Applications of transition metal complexes in the synthesis of: cyclic enediynes, estrone by Volhardt, clavicipitic acid by Hegedus.

Unit 2: Asymmetric Synthesis (M = 16)

Principles; Addition to carbonyl compounds: use of chiral substrate, chiral reagent, chiral catalyst; Stereoselective reactions of carbonyl compounds: enolate formation, alkylation, asymmetric aldol reactions; Stereoselective reactions of alkenes: Diels-Alder reaction, sigmatropic rearrangement, stereoseletive hydrogenation, epoxidation, hydroxylation, aminohydroxylation, cyclopropanation; Kinetic resolution; Asymmetric synthesis of menthol (Takasago), crixivan (Merck)

Unit 3: Synthesis of complex and biologically important molecules Applying Modern reagents and methodologies (M = 17)

A. **Organic synthesis**: (i) Target-oriented synthesis – natural products, designed molecules (ii) Method-oriented synthesis – reagents, catalysts, synthetic strategies and tactics. Retrosynthetic analysis: Selected total synthesis of natural products like Taxol, Tetracycline antibiotics etc.

B. **Synthetic methodology and strategy of few compounds**: (i) cationic cyclisations: progesterone (Johnson) (ii) radical cyclisations: synthesis of hirsutene (Curran) (iii) pericyclic reactions: endiandric acids (Nicolaou); (iv) Photochemical reactions: strained compounds (isocomene by Pirrung) (v)aldol reactions: Prelog-Djerassi lactone; (vi) carbene reactions: making cyclopropanes (vii) biomimetic strategy: carpanone (Chapman) (viii) solid-supported reagents, solid phase synthesis: plicamine (Ley) (ix) combinatorial synthesis etc.

References:

1. Organic Chemistry, Vol. II - I. L. Finar, ELBS
2. Organotransition Metal Chemistry: Applications to Organic Synthesis - S. G. Davis, Pergamon
3. Transition Metals in the Synthesis of Complex Organic Molecules - L. S. Hegedus, USB
4. The Organometallic Chemistry of the Transition Metals: R. H. Crabtree.
5. Principles And Applications Of Asymmetric Synthesis – G.-Q. Lin; Y.-M. Li; A. S. C. Chan, A John Wiley & Sons, Inc.
6. Organic Chemistry - J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2nd Ed, 2012.
7. Asymmetric synthesis: J.D. Morrison, Vol 1-5, Academic press, 1983.
8. Stereochemistry of Carbon Compounds - E.L. Eliel and S.H.Wilen, McGraw Hill Education, 2001.
9. Comprehensive asymmetric catalysis - Jacobson, E. N.; Pfaltz, A.; Yamamoto, H. Eds.), Springer 2000.
10. Asymmetric catalysis in organic synthesis: R. Noyori, Wiley-NY 1994.
11. Catalytic asymmetric synthesis: I. Ojima, VCH-NY, Pergamon, 1998.
12. Methods for the asymmetric synthesis of complex organic molecules: Daniel, J. O'Leary, Lecture Notes 2001.
13. Principles of Asymmetric Synthesis (Tetrahedron series in Organic Chemistry), R. E. Gawley, J Aube, Pergman, 1996.
14. Classics in Total Synthesis: Targets, Strategies, Methods: K. C. Nicolaou, E. J. Sorensen, Wiley, 1996.

15. Classics in Total Synthesis II - K.C. Nicolaou and S.A. Snyder Wiley-VCH.

Course Learning Outcomes: After completion of the course, the student should be able to

1. Implement the idea of Organotransition Metal Chemistry for synthesis of Organic compounds.
2. Enhance broad understanding of stereochemistry, biological relevance of isomers, resolution, importance of asymmetric synthesis using chiral auxiliary, asymmetric catalysis, chiral ligand designing etc. They will reach upto the frontier knowledge about the importance of synthesizing enantiomerically pure organic compounds and strategies available for this purpose.
3. Explore various synthetic methodologies and strategies for the preparation of complex and biologically important molecules.

Course No. CHEM 1001B (FM = 50; C = 4)
Advanced Inorganic Chemistry -II

Course Objectives: To impart the knowledge of spectroscopic analysis for inorganic systems, advance functional materials and nanomaterials

Unit 1 Spectroscopy - Applications to Inorganic Systems (M = 25) Electronic spectroscopy: Orgel diagrams, correlation between weak field and strong field terms. Tanabe-Sugano diagram, bonding parameters and structural evidences from electronicspectra of d-metal complexes, f-f transition, lanthanide and actinide spectra. Applications of IR, Raman, ESR and Mossbauer spectroscopy to inorganic and bioinorganic systems, NMR spectra: ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P NMR spectroscopy with typical examples, ^{1}HNMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and resonance shift. NQR spectroscopy: Principle, nuclear quadruple coupling constants, structural information from NQR spectra. Applications of CD and MCD; stereoselective and stereospecific effects.

Unit 2 Advanced Functional Inorganic Materials (12)

Metal complexes: with salan, salen and salophen types of ligands: synthesis, properties and applications. Supramolecular chemistry: Introduction to Metal Organic Frameworks (MOFs), design of simple and functional MOFs by postsynthetic modification, tuning of their structure, properties and various recent applications.

Unit 3 Advanced Inorganic Nanomaterials (13)

Introduction to nanomaterials, Surface area and quantum effects in nanomaterials. Conventional types of nanomaterials: carbon based, metal based, dendrimer based, and composite based. Nanomaterials synthesis and processing: Top-Down and bottom-up approach. Chemical Analysis of nanomaterials: Energy dispersive X-ray spectroscopy (EDS/EDX); Xray photoelectron spectroscopy (XPS), X-ray diffraction. Atomic absorption spectroscopy (AAS); inductively coupled plasma-atomic emission spectroscopy (ICP-AES), temperature programmed desorption (TPD); Thermogravimetric analysis (TGA) Basic concepts in surface imaging; secondary electron microscopy (SEM); scanning tunnelling microscopy (STM); transmission electron microscopy (TEM), atomic force microscopy (AFM) Optical property study: photoluminescence, FTIR, Raman spectroscopy.
Application of inorganic nanomaterials in catalysis, environmental remediation, sensing, biotechnology etc.

References

1. Inorganic Spectroscopic Methods - Alan K Brisdon.
2. Physical Methods for Chemists - R. S. Drago.
3. Fundamentals of Molecular spectroscopy - N. Banwell, E. M. McCash.
4. Inorganic Nanomaterials: Synthesis Characterization and Applications – M. Zhang.
5. Inorganic Nanoparticles: Synthesis, Applications, and Perspectives - Altavilla, E. Ciliberto.
6. The Chemistry of Nanomaterials: Synthesis, Properties and Applications - N. Rao, A. Muller, A. K. Cheetham.

Course learning outcome: After the completion of the course, the students should be able to

1. Rationalize the spectral properties of inorganic materials with appropriate theory
2. Explain the structure-property relationship of inorganic or bioinorganic systems by spectroscopic methods
3. Design the novel functional materials and analyse the characterization data
4. Explain the principle of nanosizing, design the nanomaterials and analyse the characterization data

Course No. CHEM 1001C (FM = 50; C = 4)
Advanced Physical Chemistry -II

Course Objectives: To acquire knowledge of many electron system, irreversible thermodynamics, trajectory for collision and electrode-solution interface.

Unit l Quantum Mechanics - II (M = 10)

Vector space, matrix representation of operators, Hermitian operators and matrices, Virial theorem, parity, time reversal symmetry; angular momentum operator – commutation relation, set-up and set-down operators, angular momentum operators in polar coordinates, angular momentum eigenfunctions: solutions from corresponding eigenvalue equation.
Many electron Hamiltonian, its communication with composite L^2 and Lz; spin operator and Pauli spin matrices; many electron atom and construction of wavefunction representing spectroscopic state; projection operators and their properties – projection operator technique and angular momentum.

Unit 2 Non-equilibrium phenomena (M = 15)

(a) Einstein's theory of Brownian motion; Diffusion and mobility, Perrin experiment, Determination of Avogadro number, Deduction of equation of motion for Brownian particles - Langevin's description, System bath equilibrium - fluctuation dissipation relation, General expression for mean square displacement, Probabilistic description of Brownian motion - Fokker-Planck equation; solution for free particles.

(b) Binomial, Poisson, and Gaussian distributions - generating functions, moment generating function, Characteristic Function, Cumulant Generating Function, The Central Limit Theorem.

(c) Classical Linear Response Theory, Properties of the Response Function, Causality, stationarity, impulse response, The Susceptibility, Kramers–Krönig relations, Application to a Driven Harmonic Oscillator; Quantum Linear Response Functions.; The Response Function and Energy Absorption, Relaxation of a Prepared State

Unit 3 Molecular Reaction Dynamics (M = 10)

Reaction dynamics: Introduction, molecular dynamics – intermolecular collision and its consequence; role of intermolecular potential, reaction cross-section, energy threshold, reaction probability; angular distribution in relative collision; scattering in velocity space; electronic energy transfer; experimental methods in connection with molecular dynamics; chemiluminescence; chemical laser; crossed molecular beam; photofragmentation spectroscopy.

Unit 4 Advanced Electrochemistry (M = 15)

Limitation of Debye-Hückel limiting law and its extension; Pitzer ion- interaction approach. Debye-Hückel-Onsagar (DHO) theory of electrical conduction of electrolytes, electrophoretic and relaxation effects, Wien effect, Debye-Falkenhagen effect, application of DHO theory. Limitation of DHO equation and Shedlovsky approach.

Double layer studies: nature of the double layer across electrode-solution interface, polarizable and non-polarizable electrodes, electrocapilarity (EC) – nature of EC curves, its thermodynamics, Lipmann equation, Helmholtz, Guoy- Chapman and Stern double layer models. Electron transfer reactions; fuel cells.

References:

1. Quantum Mechanics Concepts and Applications, Second Edition, - Nouredine Zettili.
2. Quantum Mechanics in Chemistry – G. C. Schatz and M. A. Ratner.
3. Quantum Chemistry, 7 th Edition, - Ira N. Levine.
4. Introduction to quantum mechanics - David J. Griffiths.
5. R. K. Pathria - Statistical Mechanics.
6. Einstein A 1956 Investigations on the theory of Brownian movement edited by R. Furth (Dover, NewYork) [Papers I and Chandrasekhar S 1943 Stochastic problems in Physics and Astronomy, Rev. Mod. Phys.15 1
7. Chemical Dynamics in Condensed Phases - Nitzan, A.
8. Gardiner, Handbook for stochastic methods: for physics, chemistry and natural sciences
9. Modern Electrochemistry 1: Ionics - J.O.M. Bockris; A. K. N. Reddy (Springer)
10. Modern Electrochemistry 2A: Fundamentals of Electrodics - J.O.M. Bockris; A. K. N. Reddy (Springer)
11. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology, and Environmental Sciences - J.O.M. Bockris; A. K. N. Reddy.

12. An Introduction to Electrochemistry - S. Glasstone.
13. Textbook of Physical Chemistry - S. Glasstone.

Course learning outcomes: After the completion of the course, the students should be able to

1. Represent quantum mechanical operators in the matrix form
2. Solve eigen value-eigen functions using matrix algebra
3. Explain Brownian motion in velocity space, properties of thermodynamic fluctuations, laws of irreversible thermodynamics and their application.
4. Express for energy dependent collision cross section, classical trajectory for bimolecular collision with angular distribution of products and concept of opacity function, chemical laser.
5. Describe quantitatively how the activity coefficients of electrolyte solutions upto saturation vary with concentration.
6. Explain the theory of conduction of electricity in electrolyte solutions.
7. Explain the behaviour of electrical double layers

Course No. CHEM 1002A (FM = 50; C = 4)
Advanced Organic Chemistry -III

Course Objectives: This course aims to (i) provide critical knowledge about target-oriented synthesis of complex heterocyclic scaffold and medicinally important molecules (ii) deal with the essentials of chemistry and biology of important class of biomolecules: nucleic acids, proteins and enzymes enabling the students to learn more advanced topics of biology including structural biology, biotechnology, genomics and proteomics etc.

Unit 1: Advanced Heterocyclic Chemistry (Two and more heteroatom) (M = 17)

Synthesis and reactivity of 5,6-membered rings containing two heteroatoms, pyrimidines and purines. Introduction to chemistry of azepins, oxepins, thiepins and their analogues; phosphorous and selenium containing heterocycles with the use of modern reagents. ANRORC and Vicarious nucleophilic substitutions in heterocycles.

Unit 2: The molecules of life (M = 16)

Introduction: The molecules of life – nucleic acids, proteins and enzymes, carbohydrates, lipids. Mechanism in biological chemistry: (i) Mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A (ii) Enzyme catalysed reactions – examples of nucleophilic displacement on a phosphorus atom, coupling of ATP cleavage to endergonic processes, proton transfer reactions to and from carbon (iii) Mechanism of reactions catalysed by cofactors including coenzyme A, NAD^+, NADH, FAD and thiamine pyrophosphate; Chemical synthesis of peptides and proteins; Use of enzymes in organic synthesis; Structural analysis of proteins; Protein folding; Biotechnological applications of enzymes: Enzyme purification, immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology.

Unit 3: Chemistry of Medicinally Important Molecules (M = 17)

Bacterial and animal cells, antibacterial agents – mechanism with reference to β-lactam antibiotics; General method of synthesis of β-lactam ring: synthesis ofpenicillin, 6-APA, cephalosporin, 7-ACA; Morin – Jackson rearrangement; Structure-activity relationship of penicillin. New generation antibiotics / antibacterial agents: Synthesis and mechanism of action of (i) fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secretion inhibitor – omeprazole (vi) drug for impotency – sildenafil etc.

References:

1. Heterocycles in Organic Synthesis - A.I. Meyers, Wiley
2. Heterocyclic Chemistry - J.A. Joule and K. Mills, Blackwell
3. Heterocyclic Chemistry - T.L. Gilchrist, Wiley
4. Organic Chemistry, Vol. I and II - I. L. Finar, ELBS
5. Lehninger Principles of Biochemistry: David L. Nelson, Michael M. Cox.
6. Fundamentals of Biochemistry: Life at the Molecular Level: Donald Voet, Judith G. Voet, Charlotte W. Pratt.
7. Burger's Medicinal Chemistry, Drug Discovery and Developments (Vol 1-8) by Burger and Burger
8. The Organic Chemistry of Drug Design and Drug Action - R. B. Silverman
9. Top Drugs: Their History, Pharmacology and Synthesis - Ji Jack Li
10. Beta lactams (Vol I and II) - A.K. Bose and M. S. Manhas
11. Medicinal Chemistry - G. L. Patrick

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explore advanced Heterocyclic Chemistry of sulphur, selenium, oxygen, nitrogen containing organic compounds including puring, pyrimidines.
2. Develop the knowledge of the molecules of life – such as nucleic acids, proteins and enzymes, carbohydrates, lipids and their Mechanism in biological chemistry.
3. Use sophisticated methods of preparation to prepare modern medicinally important molecules

Course No. CHEM 1002B (FM = 50; C = 4)
Advanced Inorganic Chemistry -III

Course Objectives: To impart the knowledge of inorganic reaction mechanisms, bioinorganic chemistry and advance materials for energy storage

Unit 1 Inorganic Reaction Mechanism (M = 25)

Mechanism of substitution reactions: Solvent exchange, aquation, anation, base hydrolysis, acid catalysed aquation, pseudo-substitution. Four board classes of mechanism of substitution – 'D', 'A', 'Ia' and 'Id' Mechanism of isomerisation reaction–linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemisation, Ray– Dutta and Bailar twist mechanisms. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, selfexchange reactions. Outer sphere and inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Inorganic Photochemistry: Excitation modes in transition metal complexes, fate of photo excited species; photochemical processes: Photosubstitution and photoelectron transfer reactions in Co, Cr and Rh-complexes.

UNIT 2 Advance materials for energy storage (M=10)

Classifications of energy storage devices-batteries and supercapacitors; Energy storage mechanisms; Materials design for energy storage; Cyclic voltammetric and electrochemical impedance spectroscopic characterizations for energy materials; Classification of batteries-primary and secondary; Mechanisms of lead-acid and lithium-ion batteries; Classifications of supercapacitors; Electrical double layer capacitors; pseudocapacitors; hybrid capacitors; Applications of energy storage devices

Unit 3 Bioinorganic Chemistry (M = 15)

Uniqueness of metal ion as bioelements. Interaction of metal ions with biomolecules, Metalloproteins and metalloenzymes Oxygen uptake proteins:- hemoglobin and myoglobin; Electron transport proteins: – cytochromes (specially cytochrome C), ferridoxins; metalloenzymes: – catalase, peroxidase, superoxide dismutase (SOD), cytochrome C oxidase, carbonic anhydrase, carboxypeptidase; respiratory electron transport chain and photosynthetic electron transport chain, Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs, metal dependent diseases.

References

1. Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications - B. E. Conway
2. Lithium-Ion Batteries: Science and Technologies - M. Yoshio, R. J. Brodd and A. Kozawa
3. Lead-Acid Batteries: Science and Technology - D. Pavlov
4. Bioinorganic Chemistry - Asim K Das
5. Selected Topics in Inorganic Chemistry - W. U. Malik, G. D. Tuli, R. D. Madan.

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain the mechanistic pathway of inorganic reactions for coordination compounds
2. Explain functioning of important enzymes and proteins in our body and have ideas of metal-based drugs and their side effects.
3. Have ideas of metal induces pollution to environment & living system and some possible remedy.
4. Explain the fundamental concepts of batteries and supercapacitors
5. Design the optimized hybrid device based on the targeted application

Course No. CHEM 1002C (FM = 50; C = 4)
Advanced Physical Chemistry -III

Course Objectives: To impart knowledge about advance quantum chemistry, selection rule, symmetry operators in vector space and utilization of the great orthogonality theorem.

Unit 1 Quantum mechanics - III (M = 15)

Perturbation theory (PT) – Rayleigh-Schrödinger PT for non-degenerate states theorem, some simple applications: expression for polarizability, ground state of helium atom; degenerate state PT – Stark effect, lifting of degeneracy by application of a magnetic field (e.g., the $^1P1$ state of helium atom) variation method – Euler variation, principle and Rayleigh-Ritz variation theorem, applications. Hückel Molecular Orbital theory for π-conjugated system.

Quantum chemistry: Born-Oppenheimer approximation, theories of valence, the MO and VB methods for H2 molecule – their relative merits, dissociation curve, excited state, configuration interaction.

Many electron systems – its characteristics, independent particle model (IPM), Hartree and Hartree-Fock methods for closed shell (elementary ideas). Basics of Density Functional Theory.

Unit 2 Quantum mechanics and spectroscopy (M = 20)

Time dependent perturbation theory – semiclassical treatment of interaction of matter with radiation, first and second order effects, Fermi golden rule, selection rule, selection rule for vibrational spectra, anharmonicity correction by perturbation – appearance of overtones; selection rule for rotational spectra, nucleur spin and rotational energy levels, stark effect revisited.

Raman scattering: selection rule for rotational and vibrational raman spectroscopy.

Quantum mechanical theory of magnetic resonance; Bloch equations and their solutions; theories of shielding – diamagnetic and paramagnetic shielding.

Unit 3 Advanced Group theory (M = 15)

Representation of symmetry operator – transformation of basis vector, general vector and functions under symmetry operations; symmetry transformation of operators and operator equation; invariance of the Hamiltonian under symmetry operation; vector space and representation theory, reducible and irreducible representations, concepts of classes and character; Wave functions as the basis of irreducible representations.

Great orthogonality and related theorems, construction of character table, reduction formula and projection operators, direct product representation, theorem on vanishing matrix elements; applications of the projection operator technique and the direct product representation.

References

1. Quantum Mechanics Concepts and Applications, Second Edition, - Nouredine Zettili.
2. Quantum Mechanics in Chemistry - G. C. Schatz and M. A. Ratner.
3. Quantum Chemistry, 7 th Edition, - Ira N. Levine.
4. Introduction to quantum mechanics - David J. Griffiths.
5. Molecular Spectroscopy - Ira N. Levine.
6. Molecular Quantum Mechanics - P. W. Atkins, R. S. Friedman.
7. Chemical Applications of Group Theory - F. A. Cotton.
8. Group Theory and Chemistry - D. M. Bishop.

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain the concept of Perturbation theory for degenerate and nondegenerate states,
2. Apply the approximation methods to solve the Schrodinger equation of many electron systems and their application for to describe the concept of bonding.
3. Describe selection rule for rotational, vibrational and vibrational Raman spectroscopy, concept of Bloch equations and their solutions.
4. Express matrix representation of operators using vector space, reducible, irreducible and direct product representation.
5. Apply projection operator technique in molecular system.

Course No. CHEM 1003 (FM = 50; C = 4)
Seminar/Review and Grand Viva

Course Objective: To provide training on the scientific presentation and group discussion skills which will help them to prepare for job interviews in academia and industries.

1. Poster presentation/Seminar/Review (M = 30)
2. Grand viva (M = 20)

Course learning outcomes: On completion of the course, the students should be able to

1. Present scientific topics in an organized manner
2. face the job interviews in a confident manner.

Course No. CHEM 1091 & CHEM 1092 (FM = 50 + 50)
Project dissertation, presentation, defense and proposal

Course Objective: To provide training for literature survey, experimental and theoretical research work, instrumental techniques and their operational procedure useful for their employability in industry and academia and also to orient them for future PhD programs.

Course No. CHEM 1091 (FM=50)
Project dissertation

The students will be carrying out a project work of 4 months duration in any of the research laboratory in the Department of chemistry according to their interest and availability of the position. This dissertation has to be submitted in the form of a thesis. The M. Sc. thesis will have two chapters. The chapter 1 will contain detail literature survey on the project topic and chapter 2 will contain the origin of the project work, methodology, results and discussion and conclusions. The training and the M. Sc. thesis of these students will then be evaluated.

Course No. CHEM 1092 (FM=50)

Project presentation, defense, proposal

1. Project presentation and defense (M = 40)

2. Short project proposal (M =10)

Course learning outcomes: On completion of the course, the students should be able to

1. Explore new areas of research in both chemistry and allied fields of science and technology
2. Perform literature survey for the research topic of his/her area of expertise.
3. Rationalize the research gap for new innovation.
4. Comprehend expertise for writing the research reports.
5. Expose safe laboratory practices by handling high end equipment and chemical reagents.