

SEMESTERWISE COURSE STRUCTURE & SYLLABUS FOR
M.Sc. CHEMICAL SCIENCES

(Two years course with four semesters)

Total credits = 72

School of Chemical Sciences

Central University of Gujarat

Gandhinagar – 382030

SEMESTER I

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-401	Inorganic Chemistry I	1	3
CHE-402	Physical Chemistry I	1	3
CHE-403	Organic Chemistry I	1	3
CHE-404	Analytical Chemistry I	1	3
CHE-441	Physical Chemistry Laboratory I	3	2
CHE-442	Inorganic Chemistry Laboratory I	3	2
CHE-443	Organic Chemistry Laboratory I	3	2
Total Credits (A)			18

SEMESTER- II

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-451	Inorganic Chemistry II	1	3
CHE-452	Physical Chemistry II	1	3
CHE-453	Organic Chemistry II	1	3
CHE-454	Analytical Chemistry II	1	3
CHE-491	Physical Chemistry Laboratory II	3	2
CHE-492	Inorganic Chemistry Laboratory II	3	2
CHE-493	Organic Chemistry Laboratory II	3	2
Total Credits (B)			18

SEMESTER- III

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-501	Inorganic Chemistry III	1	3
CHE-502	Physical Chemistry III	1	3
CHE-503	Organic Chemistry III	1	3
CHE-504	Analytical Chemistry III	1	3
CHE-541	Organic Chemistry Laboratory III	3	2
CHE-542	Physical Chemistry Laboratory III	3	2
CHE-543	Inorganic Chemistry Laboratory III	3	2
Total Credits (C)			18

SEMESTER- IV

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-551	Inorganic Chemistry IV	1	3
CHE-552	Physical Chemistry IV	1	3
CHE-553	Organic Chemistry IV	1	3
CHE-554	Analytical Chemistry IV	1	3
CHE-591	Organic Chemistry Laboratory IV	3	1
CHE-592	Physical Chemistry Laboratory IV	3	1
CHE-593	Inorganic Chemistry Laboratory IV	3	1
CHE-594	Project	3	3
Total Credits (D)			18
Grand Total Credits (A+B+C+D)			72

PROJECT

A student is free to pick up a topic for the project at the beginning of Semester III. The student is expected to complete the major literature survey during the Semester III and present a tentative research plan at the end of Semester III. The candidate will do the experimental work during Semester IV under the supervision of a guide and submit the results in the form of a thesis at the end of Semester IV. The project will be evaluated by the concerned guide.

Course Code: Core -1, Optional - 2, Filed Work / Practical - 3, Non-Credit - 4, Repeat - 5

SEMESTER I

COURSE NO.	COURSE TITLE	COURSE CODE	CREDIT
CHE-401	<p>Inorganic Chemistry I</p> <p>UNIT-I <i>Symmetry and group theory I:</i> Point symmetry operations, groups and group multiplication tables, similarity transformation and conjugate classes, identification of point groups and stereographic projection, representation of symmetry operators and groups; characters of symmetry operators in a representation, invariance of character under similarity transformation, rules (without derivation) for construction of character tables with illustrations, symmetry elements and symmetry operations of the Platonic solids, symmetry of the fullerene [60] structure.</p> <p>UNIT-II <i>Coordination chemistry:</i> Bonding, stereochemistry and structure: Crystal field theory, crystal field diagram, ligand field theory, molecular orbital theory and angular overlap model; spectral properties, vibronic coupling, intensity stealing, band broadening, spectrochemical series, nephelauxetic series; magnetic properties; structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibria. <i>Cluster compounds:</i> Introduction, clusters in elemental states, cluster classification, skeletal electron (Elm) counting, higher boron hydrides-structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, chevrel compounds, infinite metal chains, cluster-surface analogy.</p> <p>UNIT-III <i>Bioinorganic chemistry:</i> Transition elements in Biology-their occurrence and function, active site structure and function of metalloproteins and metalloenzymes. O₂ binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocyanin & hemerythrin) their co-ordination, geometry and electronic structure.</p> <p>Electron transfer proteins- active site structure and functions of ferredoxin, rubridoxin and cytochromes and their comparison. Vitamins B12 and cytochrome P450 and their mechanism of actions. Metals in medicine-therapeutic applications of cis-platin, radioisotopes and MRI agents. Toxicity of metals; Cd, Hg and Cr toxic effects with specific examples.</p> <p><u>Reference Books:</u></p> <ol style="list-style-type: none"> 1. F. A. Cotton, <i>Chemical Applications of Group Theory</i>, 3rd Edn Reprint, John Wiley and Sons, New York, 1999. 2. A. Vincent, <i>Molecular Symmetry and Group Theory</i>, John Wiley and Sons, New York, 1998. 	1	3

	<ol style="list-style-type: none"> 3. R. McWeeney, <i>Coulsons' Valence</i>, 3rd Edn, Oxford University Press, Oxford, 1979. 4. T. A. Albright, J. K. Burdett and M. H. Whangbo, <i>Orbital Interactions in Chemistry</i>, Wiley, New York, 1985. 5. K. Fukui and Fujimoto, <i>Frontier Orbital and Reaction Paths</i>, World Scientific, Singapore, 1995 6. G. Wulfsberg, <i>Inorganic Chemistry</i>, Viva Books Private Ltd., New Delhi, 2001. 7. D. F. Shriver, P. W. Atkins and C. H. Langford, <i>Inorganic Chemistry</i>, Oxford University Press, New York, 1990. 8. B. Douglas, D. McDaniel and J. Alexander, <i>Concepts and Models of Inorganic Chemistry</i>, 3rd Edn, John Wiley and Sons, Inc., New York, 2001. 9. J. E. Huheey, E. A. Keiter and R. L. Keiter, <i>Inorganic Chemistry: Principles of Structure and Reactivity</i>, 4th Edn, Harper Collins College Publishers, New York, 1993. 10. T. P. Fehlner, J. –F. Halet and J. –Y. Saillard, <i>Molecular Clusters — A Bridge to Solid State Chemistry</i>, Cambridge University Press, Cambridge, 2007. 11. M. Driess and H. Noth (Eds.), <i>Molecular Clusters of the Main Group Elements</i>, Wiley-VCH, Weinheim, 2004. 12. D. M. P. Mingos and D. J. Wales, <i>Introduction to Cluster Chemistry</i>, Prentice Hall, New York, 1990. 13. D. M. P. Mingos (Ed.), <i>Structural and Electronic Paradigms in Cluster Chemistry</i>, Springer, Berlin, 1997. 14. D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds.), <i>The Chemistry of Metal Cluster Complexes</i>, VCH, New York, 1990. 15. P. Braunstein, L. A. Oro and P. R. Raithby (Eds.), <i>Metal Clusters in Chemistry</i>, Wiley-VCH, Weinheim, 1999. 16. M. H. Chisholm (Ed.), <i>Early Transition Metal Clusters with π-Donor Ligands</i>, VCH, New York, 1995. 17. K. J. Klabunde, <i>Free Atoms, Clusters and Nanoscale Particles</i>, Academic Press, New York, 1994. 18. J. G. Verkade, <i>A Pictorial Approach to Molecular Bonding</i>, 2nd Edn, Springer-Verlag, New York, 1997. 19. O. Kahn, <i>Molecular Magnetism</i>, VCH, New York, 1993. 20. A. Das and G. N. Mukherjee, <i>Elements of Bioinorganic Chemistry</i>, 2nd Edn, U. N. Dhur and Sons, Kolkata, 2002. 21. I. Bertini, H. B. Gray, S. J. Lipperd and J. S. Valentine, <i>Bioinorganic Chemistry</i>, Viva Books Pvt. Ltd., New Delhi, 1998. 22. W. Kaim and B. Schwederski, <i>Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life</i>, Wiley, New York, 1994. 23. S. J. Lippard and J. M. Berg, <i>Principles of Bioinorganic Chemistry</i>, University Science Books, Mill Valley, CA, 1993. 24. P. M. Harrison and R. J. Hoare, <i>Metals in Biochemistry</i>, Chapman and Hall, 1980. 25. C. A. McAuliffe (Ed) <i>Techniques and Topics in Bioinorganic Chemistry</i>, Halsted, New York, 1975. 26. R. W. Hay, <i>Bioinorganic Chemistry</i>, Ellis Horwood, Chichester, New York, 1984. 		
CHE-402	<p>Physical Chemistry I</p> <p>UNIT-I</p> <p><i>Quantum chemistry:</i> Summarization of the results of some experiments – black-body radiation, photoelectric effect, Davison and Germer experiment, Franck-Hertz experiment, Young's double slit experiment; identification of classical and quantum systems, Bohr's correspondence principle with examples; postulates of quantum mechanics, properties of wave functions, operators and related theorems</p> <p><i>Mathematical methods:</i> Elementary vector calculus, equation of continuity of fluid motion, diagonalisation of square symmetric matrices (real elements) by Jacobi method; coordinate transformation</p>	1	3

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UNIT-II

Thermodynamics and statistical mechanics: Introduction to thermodynamics laws & variables, Concept of entropy, reversible and irreversible processes, Clausius inequality, Free energies, Criteria of spontaneity. Fundamental equations for open systems, Partial molar quantities and chemical potential, Gibbs-Duhem equation, Real gases and fugacity. Thermodynamics of ideal and non-ideal solutions: Liquid-liquid solutions, liquid-solid solutions, multicomponent systems and excess thermodynamic properties, Activity of ideal, regular and ionic solutions. Strong electrolytes, Debye-Huckel limiting law and its extensions, activity coefficients and ionic strength, Applications of Debye-Huckel Theory. Thermodynamic equation of state. Phase behavior of one and two component systems, Ehrenfest classification of phase transitions.

Statistical Thermodynamics: Concept of ensembles, Canonical ensemble, Boltzmann distribution, Thermodynamic quantities and canonical partition function. Grand canonical ensemble, Fermi-Dirac and Bose-Einstein distributions. Molecular partition functions, Translational, rotational and vibrational partition functions. Ideal monoatomic and diatomic gases, Classical partition functions, thermodynamic properties, Equi-partition theorem, Chemical equilibrium. Real gases, intermolecular potential and virial coefficients. Debye and Einstein theory of heat capacity of solids. Structure and thermal properties of liquids, Pair correlation functions. Linear response theory, Irreversible processes, Onsager's law, Entropy production, Non-equilibrium stationary states.

UNIT-III

Principles of molecular spectroscopy: Electromagnetic spectrum and molecular processes associated with the regions; rotational spectra: classification of molecules into spherical, symmetric and asymmetric tops; diatomic molecules as rigid rotors – energy levels, selection rules and spectral features, isotope effect, intensity distribution, effect of non-rigidity on spectral features; vibrational spectra of diatomics: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: origin; selection rules; P, Q and R branches; Raman spectra: origin, selection rules, rotational and vibrational Raman spectra of diatomics; NMR spectra: theory, relaxation process, instrumentation, chemical shift and shielding, factors contributing to magnitude of shielding, spin interactions – its origin, equivalent protons, qualitative idea of energy levels of AX and A₂ systems, a few representative examples

Reference Books:

1. P. Atkins and J. Paula, Physical Chemistry, 8th Edition, Oxford University Press, Oxford 2006.
2. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2004.
3. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford 2007.

	<ol style="list-style-type: none"> 4. D. A. McQuarrie, <i>Statistical Mechanics</i>, University Science Books, California (2005). 5. B. Widom, <i>Statistical Mechanics - A Concise Introduction for Chemists</i>, Cambridge University Press 2002. 6. D. Chandler, <i>Introduction to Modern Statistical Mechanics</i>, Oxford University Press 1987. 7. G. W. Castellan, <i>Physical Chemistry</i>, 3rd Edn, Narosa Publishing House, 1995. 8. I. N. Levine, <i>Physical Chemistry</i>, Tata McGraw-Hill, 1978. 9. G. K. Vemulapalli, <i>Physical Chemistry</i>, Prentice-Hall, India, 1997. 10. R. S. Berry, S. A. Rice and J. Ross, <i>Physical Chemistry</i>, Oxford University Press, Oxford, 2000. 11. P. W. Atkins, <i>Physical Chemistry</i>, Oxford University Press, Oxford, 1998. 12. H. Eyring, J. Walter and G. F. Kimball, <i>Quantum Chemistry</i>, Wiley, New York, 1944. 12 13. A. K. Chandra, <i>Introductory Quantum Chemistry</i>, Tata McGraw-Hill Publishing Co, New Delhi, 1989. 14. F. L. Pilar, <i>Elementary Quantum Chemistry</i>, Tata McGraw-Hill, 1990. 15. P. W. Atkins, <i>Molecular Quantum Mechanics</i>, Clarendon Press, Oxford, 1980. 16. E. Merzbacher, <i>Quantum Mechanics</i>, John Wiley and Sons, 1970. 17. L. I. Schiff, <i>Quantum Mechanics</i>, McGraw-Hill, 1985. 18. L. Pauling and E. B. Wilson, <i>Introduction to Quantum Mechanics</i>, McGraw-Hill, 1939. 19. C. N. Banwell and E. M. McCash, <i>Fundamentals of Molecular Spectroscopy</i>, 4th Edn, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 1994. 20. G. M. Barrow, <i>Introduction to Molecular Spectroscopy</i>, McGraw-Hill International Book Company, Tokyo, 1982. 21. K. Denbigh, <i>Principles of Chemical Equilibrium</i>, Cambridge University Press, Cambridge, 1981. 22. N. A. Gokcen and R. G. Reddy, <i>Thermodynamics</i>, Plenum Press, New York, 1996. 23. I. M. Klotz and R. M. Rosenberg, <i>Chemical Thermodynamics</i>, John Wiley, New York, 1994. 24. F. Reif, <i>Fundamentals of Statistical and Thermal Physics</i>, McGraw-Hill, 1965. 		
CHE-403	<p>Organic Chemistry I</p> <p>UNIT-I <i>Nomenclature:</i> IUPAC nomenclature of organic molecules including regio- and stereoisomers. <i>Principles of stereochemistry:</i> Molecular symmetry and chirality; stereoisomerism: definitions, classifications; Configuration and conformation; relative and absolute configuration; determination of relative configuration: Prelog's rule, Cram's rule (Felkin modification), and Sharpless rule; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction; conformations of acyclic and cyclic system (3 to 8 membered rings), fused (5/5 & 6/6), spiro and bridged bicyclo systems; stability, reactivity and mechanism; allylic strain; reactions of 5/6-membered ring containing one or more trigonal carbon(s). <i>Quantitative relationship between structure and reactivity:</i> Linear free energy relations: Hammett equation; equilibria and rates in organic reactions; separation of polar, steric and resonance effects: Taft equation, Grunwald -Winstein equation</p> <p>UNIT-II <i>Infrared Spectroscopy:</i> Concept of vibrational spectra, stretching and bending vibrations, application identification of functional groups, applications in sequence of organic synthetic reactions and in the structure elucidation of simple organic molecules, FTIR <i>Mass spectrometry:</i> Basic principles, Electron impact mass</p>	1	3

spectroscopy, ionization techniques, low and high resolution, isotope abundance, molecular ion, fragmentation processes of organic molecules, fragment ions of odd and even electron types, rearrangement ions, factors affecting cleavage patterns, mass marking techniques, McLafferty rearrangement, deduction of structure using mass spectral fragmentation, FAB-Mass, high resolution MS, soft ionization methods, EI-MS and MALDI-MS, illustrative examples from macromolecules/supramolecule, inorganic, coordination and organometallic compounds.

UNIT-III

UV-Visible spectroscopy: Transitions, vacuum ultraviolet, applications in conjugated dienes, some correlation studies, trienes, polyenes, steroids and triterpenoids, stereochemical applications, α,β -unsaturated carbonyl compounds; solvent effect, applications in aromatic and heterocyclic compounds

NMR: spin $\frac{1}{2}$ nuclei, (^1H , ^{13}C , ^{31}P and ^{19}F), Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ , inductive and anisotropic effects on chemical shift, chemical and magnetic equivalence of spins, spin-spin coupling, coupling constant J, first order patterns, second order effects, physical significance of AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. ^{13}C NMR, introduction to FT technique, relaxation phenomena, NOE effects, restricted rotation (DMF, DMA), cyclohexane ring inversion. Multinuclear NMR of Si, F and P nuclei; structure of inorganic molecules, MRI and application in organic molecules

Reference Books:

1. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn., Plenum Press, New York, 2001.
2. I.L. Finar, *Organic Chemistry*, Vol I, 6th Edn., Addison Wesley Longman, London, 1998.
3. I.L. Finar, *Organic Chemistry*, Vol II, 5th Edn., ELBS, London, 1995.
4. W. J. I. Noble, *Highlights of Organic Chemistry*, MerceL Dekker, 1974.
5. E.L. Eliel, S.H. Wilen and L.N. Mander, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.
6. D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn., Wiley Eastern, New Delhi, 1993.
7. W. Kemp, *Organic Spectroscopy*, 3rd Edn., McMillan, Hong Kong, 1991.
8. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5th Edn., Tata McGraw-Hill, New Delhi, 2005.
9. J. R. Dyer, *Applications of Absorption Spectroscopy of Organic compounds*, 2nd print Prentice_Hall, New Jersey, 1971. 10
10. R. M. Silverstein and F. Webster, *Spectrometric Identification of Organic Compounds*, 6th Edn., John Wiley, New York, 1998.
11. K. Biemann, *Mass Spectrometry – Application to Organic Chemistry*, McGraw-Hill, New York, 1962.
12. H. Budzikiewicz, C. Djerassi and D.H. Williams, *Mass Spectrometry of Organic Compounds*, Holden-Day, 1967.
13. R.C. Banks, E.R. Matjeka and G. Mercer, *Introductory Problems in Spectroscopy*, Benjamin/Cumings Publishing Co., 1980.
14. R.T. Morison, and R. N. Boyd, *Organic Chemistry*, 6th Edn., Prentice-Hall India Private Ltd., New Delhi, 1992.
15. J. Barker, *Mass Spectrometry*, 2nd Edn., John Wiley, New York, 2000.
16. K. Downard, *Mass Spectrometry: A Foundation Course*, Royal Society of Chemistry, UK, 2004.

	17. G. Siurdek, <i>The Expanding Role of Mass Spectrometry in Biotechnology</i> , MCC Press, San diego, 2004 18. C. Dass, <i>An Introduction to Biological Mass Spectrometry</i> , Wiley, USA, 2002.		
CHE-404	<p>Analytical Chemistry I</p> <p>UNIT-I <i>Standard data and data processing:</i> Errors, determinant, constant and indeterminate, minimisation of errors, accuracy and precision, central limit theory. Distribution of random errors. Average deviation and standard deviation, variance and confidence limit. Significance figures and computation rules, Least square method, polynomial regression and correlation analysis, mean deviation and standard deviation, Gaussian distribution. Validation Qualification, validation and calibration of equipment. Harmonised protocols for the adoption of standardized analytical methods and for the presentation of their performance characteristics. Methods of sampling: samples size.</p> <p>UNIT-II <i>Separation techniques:</i> Introduction, concept, common separation techniques, working principles, application, and limitation. <i>Solvent extraction:</i> principle, distribution ratio and partition coefficient, successive extraction and separation; different methods of extraction systems; Craig extraction and counter current distribution; problems.</p> <p>UNIT-III <i>Chromatography:</i> general principle; classification, mathematical relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, elution in column chromatography: band broadening and column efficiency; van Deemter equation; column resolution, numerical problems, gas chromatography, high performance chromatography and supercritical fluid chromatography: principles, methods, comparison and applications; thin-layer chromatography, size-exclusion chromatography, ion chromatography and capillary electrophoresis: principles, methods and applications</p> <p>Reference Books:</p> <ol style="list-style-type: none"> 1. Analytical Chemistry: (J.W)G. D. Christain 2. Introduction to chromatography: Bobbit 3. Instrumental Methods of analysis (CBS)-H. H. Willard, L. L. Mirrit, J. A. Dean 4. Instrumental Methods of Analysis: Chatwal and Anand 5. Instrumental Methods of Inorganic Analysis (ELBS):A. I. Vogel 6. Chemical Instrumentation: A Systematic approach-H. A. Strobel 7. Principal of Instrumental Analysis-D. Skoog and D. West 8. W. Dennes Pocklington Pure & Applied Chemistry, 1990, 62(1), 149-162 	1	3
CHE-441	<p>Physical Chemistry Laboratory I</p> <ol style="list-style-type: none"> 1. Simultaneous determination of surface tension and viscosity with Survismeter and statistical analysis of the data (standard deviation, error, precision, and accuracy). 2. Determination of molecular weight of the polymer by viscosity method. 	3	2

	<ol style="list-style-type: none"> 3. Identification of emulsifier and demulsifier of crude oil with Survismeter. 4. Separation techniques involving ion exchange and solvent extraction 		
CHE-442	Inorganic Chemistry Laboratory I <ol style="list-style-type: none"> 1. Experiments on quantitative estimation: analysis of selected ores, minerals and alloys 2. Synthesis and identification of inorganic coordination compounds: 3. Separation of optical isomers of cis-[Co(en)₂Cl₂]Cl. 4. Determination of Cr(III) complexes. [Cr(H₂O)NO₃]NO₃.3H₂O, [Cr(H₂O)Cl₂]Cl.2H₂O, Cr(acac)₃ 	3	2
CHE-443	Organic Chemistry Laboratory I <ol style="list-style-type: none"> 1. Separation and identification of ternary mixtures of organic compounds. 2. Synthesis of organic compounds involving important chemical reactions: Bromination, sulfonation, nitration, diazotisation, Beckmann transformation, photochemical reaction, Sandmeyer reaction, pinacol-pinacolone rearrangement and confirmation by preparation of derivatives. 3. Spectrophotometric identification of simple organic compounds (IR, NMR, Mass and UV-Vis) 4. Introduction to non-breakable sodium ignition apparatus (NOSIA) in qualitative analysis of organic compounds. 	3	2

SEMESTER- II

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-451	Inorganic Chemistry II UNIT I <i>Chemistry of elements:</i> Design and synthesis, geometric and electronic structures, stereochemistry and bonding, reactivity and reaction pathways of various coordination compounds of transition and non-transition metal ions with halide, pseudohalide, aquo, hydroxo, oxo, carboxylate, amine, amide, polypyridine, azoimine, phosphine, carbonyl, nitrosyl, dioxolene, azophenol, macrocycle, Schiff base and their mixed mono-, bi-, and polynuclear complexes; a closer look at the applications of coordination molecules in different fields of chemistry and allied fields. UNIT II <i>Solid state chemistry:</i> Bonding in metals, ionic, covalent and hydrogen bonded solids; perovskite, ilmenite and rutile; spinel and inverse spinel, silicates: pyroxene, amphibole, talc, mica, clay, zeolite, ultramarine; crystal synthesis and defects, non-stoichiometric compounds; electronic properties of solids, conductors, semiconductors, insulators, superconductors; ferroelectricity, antiferroelectricity, piezoelectricity, liquid crystals, cooperative magnetism <i>Crystal structure:</i> translation, glide plane and screw axis; diffraction of X-rays by crystals: Laue and Bragg conditions; concept of	1	3

reciprocal lattice, crystal structure factor, systematic absence; B-zones and Fermi level in lattice, concept of particle-hole in conduction process, Band theory, theory of conductors, semiconductors and insulators

UNIT III

Organometallic chemistry: Introduction, classification, nomenclature, valence electron count, oxidation number and formal ligand charge; structure and bonding of carbonyls, nitrosyls and related pi-acids, alkyl, alkene, alkyne, π -allyl, polyene and cyclopolyene compounds; metal carbenes and carbynes, isolobal analogy, Dewar-Chatt model, oxophilicity, Agostic interaction

Reference Books:

1. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn, Pergamon, New York, 1997.
2. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, Prentice-Hall, New Jersey, 1999.
3. A. F. Holleman and E. Wiberg, *Inorganic Chemistry*, Academic Press, New York, 1995.
4. G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
5. J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall, London, 1991.
6. G. Wulfsberg, *Principles of Descriptive Inorganic Chemistry*, University Science Books, Mill Valley, CA, 1991.
7. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
8. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley and Sons, Inc., New York, 2001.
9. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edn, Harper Collins College Publishers, New York, 1993.
10. G. B. Richter-Addo and P. L. Legzdins, *Metal Nitrosyls*, Oxford University Press, New York, 1992.
11. F. A. Cotton and R. A. Walton, *Multiple Bonds Between Metal Atoms*, 2nd Edn, Clarendon Press, Oxford, UK, 1993.
12. D. L. Kepert, *Inorganic Stereochemistry*, Springer, Berlin, 1982.
13. A. von Zelewsky, *Stereochemistry of Coordination Compounds*, Wiley, New York, 1996.
14. S. P. Sinha, *Systematics and Properties of Lanthanides*, Riedel, Dordrecht, 1983.
15. J. J. Katz, G. T. Seaborg and L. R. Morss (Eds), *The Chemistry of the Actinide Elements*, Vols I and II, 2nd Edn, Chapman and Hall, London, 1986.
16. A. F. Wells, *Structural Inorganic Chemistry*, 5th Edn, Oxford University Press, Oxford, 1984.
17. D. M. Adams, *Inorganic Solids*, Wiley, New York, 1992.
18. S. R. Elliot, *The Physics and Chemistry of Solids*, John Wiley & Sons, Chichester, 1998.
19. W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds*, Dover Publications, New York, 1989.
20. M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.
21. T. C. W. Mak and G. -D. Zhou, *Crystallography in Modern Chemistry*, Wiley, New York, 1992.
22. G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 1997.
23. G. A. Jeffrey and W. Saenger, *Hydrogen Bonding in Biological Structures*, Springer, Berlin, 1991.
24. A. J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.
25. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.

	<p>26. P. Powell, <i>Principles of Organometallic Chemistry</i>, 2nd Edn, Chapman and Hall, London, 1988.</p> <p>27. G. W. Parshall, <i>Homogeneous Catalysis</i>, Wiley, New York, 1980.</p> <p>28. C. N. Satterfield, <i>Heterogeneous Catalysis in Practice</i>, McGraw-Hill, New York, 1980.</p> <p>29. J. D. Atwood, <i>Inorganic and Organometallic Reaction Mechanisms</i>, 2nd Edn, VCH, New York, 1997.</p>		
CHE-452	<p>Physical Chemistry II</p> <p>UNIT I <i>Group theory:</i> Prefactory comments on Matrices and Vectors, Representation of groups, The great orthogonality theorem and its consequences, Character Tables, Representation of cyclic groups, Wave functions as bases for irreducible representation, the direct product, identifying nonzero elements, derivation of projection operators, using projection operators to constructs SALCs.</p> <p>UNIT II <i>Quantum chemistry:</i> Degeneracy; Schrödinger equation, energy-eigen value equation, expectation value, eigenvalue and spread of observation, definition of uncertainty; equation of motion, constants of motion; exactly solvable problems: harmonic oscillator, rigid rotator, step potential and tunneling; elementary discussion of the H-atom solution, Quantum numbers, orbital and spin angular momenta of electrons, Stern-Gerlach experiment, vector atom model, term symbols (one and two optical electron systems), normal and anomalous Zeeman effect, Paschenback effect.</p> <p><i>Electrochemistry:</i> Born equation, Debye-Huckel limiting law, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods to determine, ion association: Bjerrum equation, fraction of ions associated, ion association constant; electrode kinetics: relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation.</p> <p>UNIT III <i>Chemical kinetics:</i> Theories of reaction rates: applications to uni-, bi- and ter-molecular reactions, thermodynamic formulation of reaction rate, reactions in solution – cage effect, diffusion and activation controlled reactions, dielectric effect on ion-ion reaction, electrostriction, volume of activation, effect of temperature and pressure on reaction rate, classification of reactions on the basis of volume of activation, Curtin-Hammett principle, linear free energy relationship, Hammett and Taft equation; study of fast reactions – flow process and relaxation techniques</p> <p><u>Reference Books:</u></p> <ol style="list-style-type: none"> 1. G. W. Castellan, <i>Physical Chemistry</i>, 3rd Edn, Narosa Publishing House, New Delhi, 1995. 2. R. A. Alberty and R. J. Silbey, <i>Physical Chemistry</i>, 1st Edn, John Wiley & Sons, Inc., 1995. 3. R. S. Berry, S. A. Rice and J. Ross, <i>Physical Chemistry</i>, Oxford University Press, Oxford, 2000. 4. F. A. Cotton, <i>Chemical Applications of Group Theory</i>, 3rd Edn Reprint, John Wiley and Sons, New York, 1999. 	1	3

	<ol style="list-style-type: none"> 5. A. Vincent, <i>Molecular Symmetry and Group Theory</i>, John Wiley and Sons, New York, 1998. 6. S. C. Rakshit, <i>Molecular Symmetry Group and Chemistry</i>, The New Book Stall, Kolkata, 1988. 7. Volker Heine, <i>Group Theory in Quantum Mechanics: An Introduction to Its Present Usage</i>, Dover Publication, New York, 1991. 8. H. Eyring, J. Walter and G. F. Kimball, <i>Quantum Chemistry</i>, Wiley, New York, 1944. 9. H. E. White, <i>Introduction to Atomic Spectra</i>, McGraw-Hill Kogakusha Ltd., Tokyo, 1934. 10. A. K. Chandra, <i>Introductory Quantum Chemistry</i>, Tata McGraw-Hill Publishing Co, New Delhi, 1989. 11. F. L. Pilar, <i>Elementary Quantum Chemistry</i>, Tata McGraw-Hill, 1990. 12. P. W. Atkins, <i>Molecular Quantum Mechanics</i>, Clarendon Press, Oxford, 1980. 13. E. Merzbacher, <i>Quantum Mechanics</i>, John Wiley and Sons, 1970. 14. L. I. Schiff, <i>Quantum Mechanics</i>, McGraw-Hill, 1985. 15. L. Pauling and E. B. Wilson, <i>Introduction to Quantum Mechanics</i>, McGraw-Hill, 1939. 16. P. C. W. Davies, <i>Quantum Mechanics</i>, ELBS, 1985. 17. J. L. Powell and B. Crasemann, <i>Quantum Mechanics</i>, Addison-Wesley, London, 1961. 18. D. Bohm, <i>Quantum Theory</i>, Asia Pub. House, Bombay, 1960. 19. S. Glasstone, <i>An Introduction to Electrochemistry</i>, D. Van Nostrand Company, 1962. 20. J. O'M. Bockris and A. K. N. Reddy, <i>Modern Electrochemistry</i>, Vol. I, Plenum Press, New York, 1970. 21. K. J. Laidler, <i>Reaction Kinetics</i>, Vols. I & II, Pergamon Press, London, 1970. 22. K. J. Laidler, <i>Chemical Kinetics</i>, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988. 23. L. P. Hammett, <i>Physical Organic Chemistry</i>, McGraw-Hill Book Company, New Delhi, 1970. 24. M. R. Wright, <i>Fundamental Chemical Kinetics</i>, Horwood Publishing, 1999. 25. J. Albery, <i>Electrode Kinetics</i>, Oxford Chemistry Series, Clarendon Press, Oxford, 1975. 26. G. D. Mahan, <i>Many Particle Physics</i>, Kluwer Academy, Plenum Publisher, 2000. 27. C. Kittel, <i>Introduction to Solid State Physics</i>, John Wiley & Sons, 4th Ed. 28. M. F. C. Ladd and R. A. Palmer, <i>Structure Determination by X-ray Crystallography</i>, Plenum Press, New York, 3rd Ed., 1994. 29. P. A. Cox, <i>The Electronic Structure & Chemistry of Solids</i>, Oxford University Press, 1987. 30. X. Clegg, <i>Crystal Structure Determination</i>, Oxford University Press, 2005. 		
CHE-453	<p>Organic Chemistry II</p> <p>UNIT I</p> <p><i>Aromaticity:</i> Generation and reactions of benzenoid and non-benzenoid compounds</p> <p><i>Reactive intermediates with allied organic reaction mechanism:</i> Classical and non-classical carbocations and carbanions; radicals, radical cations, radical anions, carbenes, arynes and nitrenes; general methods of generation, detection, stability, reactivity and structure of the intermediates; olefin metathesis</p> <p><i>Organic reaction mechanisms:</i> addition, elimination and substitution reactions with electrophilic, nucleophilic, radical species. Determination of reaction pathways.</p> <p><i>Carbohydrate chemistry:</i> Conformational analysis of monosaccharides (pentoses and hexoses) and relative instability ratings; anomeric effect, reverse anomeric effect and their origin; mutarotation and abnormal mutarotation; use of complexing agents: borates, phosphates and copper compound; synthesis of glycosides;</p>	1	3

polysaccharide chemistry: isolation, purification, hydrolysis, methylation and periodic oxidation, Smith degradation, Barry degradation

UNIT II

Heterocyclic chemistry: Synthesis, reactivity and uses of imidazole, pyrazole, oxazole, iso-oxazole, thiazole and iso-thiazole and their derivatives.

Name Reaction: Barbier and Grignard reaction, Barbier-Wieland degradation, Cope elimination and rearrangement, Dakin, Duff, Elbspersulphate, Nef, Pechmann, Vilsmeier reactions, ketene cycloaddition (inter and intramolecular), Pauson-Khand reaction, Palladium catalysed reactions, Click reaction.

Design of Synthesis: Retrosynthetic Analysis: Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions, donor acceptor disconnection in the carbon-carbon single bond formation, Strategies for retrosynthetic analysis, ring closing metathesis.

UNIT III

Protein chemistry: Classification on the basis of composition, structures, nutrition, and function of amino acids); biological value, digestibility co-efficient, PER and NPU; peptide bond, Pauling's studies and conclusion on peptide bond, denaturation of proteins, factors effecting denaturation, essential criteria for structure elucidation of protein; primary structure, solubility studies, amino acid analysis, molecular weight determinations (intrinsic viscosity, ultracentrifugation, gel-filtration, gel-electrophoresis), C-terminal and N-terminal amino acid determinations, secondary, tertiary and quaternary structures, factors responsible for stabilization of secondary and tertiary structures, Merifield's solid state peptide synthesis

Reference Books:

1. J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 5th Edn., John Wiley, New York, 1999.
2. S. P. McManus, *Organic Reactive Intermediates*, Academic Press, New York, 1973.
3. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn., Plenum Press, New York, 2001.
4. T. L. Gilchrist and C. W. Rees, *Carbenes, Nitrenes and Arynes*, Nelson, New York, 1973.
5. T. H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn., Harper and Row, New York, 1998.
6. I.L. Finar, *Organic Chemistry*, Vol I, 6th Edn., Addison Wesley Longmann, London, 1998.
7. I.L. Finar, *Organic Chemistry*, Vol II, 5th Edn., ELBS, London, 1995.
8. D. L. Nelson and M.M. Cox, *Lehninger: Principles of Biochemistry*, W.H. Freeman Co, London, 2005.
9. H. Neurath, *The Proteins: Composition, Structure and Function*, Vols. 1-5, Academic Press, New York, 1963.

	<p>10. J. P. Greenstein and M. Winitz, <i>Chemistry of the Amino Acids (3 Vols.)</i>, Wiley, New York, 1961.</p> <p>11. W. J. I. Noble, <i>Highlights of Organic Chemistry</i>, MerceL Dekker, 1974.</p> <p>12. S.W. Fox and J.F. Foster, <i>Introduction to Protein Chemistry</i>, John Wiley, New York, 1957.</p> <p>13. E. A. Davidson, <i>Carbohydrate Chemistry</i>, Holt, Rinehart and Winston, New York 1967.</p> <p>14. R. D. Guthrie and J. Honeyman, <i>An Introduction of Chemistry of Carbohydrate</i>, 3rd Edn., Clarendon Press, Oxford, 1988.</p> <p>15. J. Kennedy, <i>Carbohydrate Chemistry</i>, Clarendon Press, Oxford, 1988.</p> <p>16. A.R. Kartiritzky, <i>Handbook of Heterocyclic Chemistry</i>, Pergamon Press, 1986.</p> <p>17. K. Nakanishi, T. Goto, S. Ito, S. Natori and S. Nozoe, <i>Natural Products Chemistry</i>, Vol. I, Academic Press, New York, 1974.</p> <p>18. James R-Hanson, <i>Organic Synthetic Methods</i>, Royal Society of Chemistry, London, 2002. 18</p> <p>19. R.S. Ward, <i>Selectivity in Organic Synthesis</i>, John Wiley & Sons, 1999, New York.</p> <p>20. J. Clayden, N. Greeves, S. Warren and P. Wothers, <i>Organic Chemistry</i>, Oxford University Press, Oxford, 2001.</p> <p>21. J.H. Fuhrhop and G. Li, <i>Organic Synthesis, Concepts and Methods</i>, Wiley VCH, New York, 2003.</p> <p>22. R. Karritzky, <i>Handbook of Heterocyclic Chemistry</i>, Pergamon Press, London, 1986.</p>		
CHE-454	<p>Analytical Chemistry II</p> <p>UNIT I <i>Potentiometric and Ion-Selective Electrodes:</i> Introduction, principle, Electrolytic cell, Galvanic cell, Standard reduction potential, Nernst equation, pH electrode, Ion-selective electrodes, Potentiometric titration <i>Oxidation-Reduction:</i> Oxidation number, Balancing red-ox equations: inspection method, half-reaction method, ion-electron method, Equivalents; Applications: potassium permanganate, iodometry, dichromate ion, cerate ion</p> <p>UNIT II <i>Volumetric Methods of Analysis:</i> Titrimetry, volumetric, gravimetric, coulometric; Terms: standard solution, titration, equivalence point, end point, indicator, titration error, blank determination, back titration, primary standard, standardization; Establishing the concentration: direct method, standardization; Concentration terms and equations: Percent concentration, parts per million (ppm), Molarity, Normality, pX; Calculations, Back Titrations</p> <p>UNIT III <i>Thermal methods:</i> Different methods of analysis: TGA, DTA, DSC; thermogram, thermal stability of covalent and non-covalent bonds, thermal degradation, single crystal phase transformation, thermo chemiluminescence, thermometric titration, solid state reaction kinetics <i>Electroanalytical methods:</i> Electrochemical cell, electrodes: reference and indicator electrodes, membrane electrodes, electrode-solution interface layer, gas-sensing probe, electrolytic process, three electrode system; supporting electrolyte, DME; Cottrell equation, Ilkovic equation, Ilkovic-Heyrotsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, stripping voltammetry, amperometric titration</p>	1	3

	<p><i>Synthetic elements: Man-made elements: theoretical background, production and separation with special reference to actinoids and superheavy elements, chemical reaction and electronic configuration</i></p> <p><u>Reference Books:</u></p> <ol style="list-style-type: none"> 1. Y. Marcus and A. S. Kertes, <i>Ion Exchange and Solvent Extraction of Metal Complexes</i>, Wiley Interscience, 1969. 2. H. F. Walton and W. Reiman, <i>Ion Exchange in Analytical Chemistry</i>, Pergamon Press, 1970. 3. A. Tarter, <i>Advanced Ion Chromatography</i>, Wiley Interscience, New York, 1989. 4. E. Heftman, <i>Chromatography</i>, Reinhold, New York, 1969. 5. G. D. Christian, <i>Analytical Chemistry</i>, 5th Edn. Wiley, New York, 1994. 6. J. A. Dean, <i>Chemical Separation Methods</i>, Van Nostrand Reinhold, London, 1970. 16 7. D. A. Skoog, D. M. West and F. J. Holley, <i>Fundamentals in Analytical Chemistry</i>, 5th Edn, Saunders, Philadelphia, 1988. 8. S. Lindsay and J. Barnes, <i>High Performance Liquid Chromatography</i>, John Wiley, New York, 1992. 9. D. G. Peters, J. M. Hayes and G. M. Hieftje, <i>Chemical Separations and Measurements: Theory and Practice of Analytical Chemistry</i>, Saunders, Wiley Interscience, New York, 1974. 10. S. M. Khopkar, <i>Basic Concepts of Analytical Chemistry</i>, Wiley Eastern Ltd., New Delhi, 1998. 11. S. E. Manahan, <i>Environmental Chemistry</i>, Lewis Publishers, Boston, 1991. 12. J. H. Seinfeld, <i>Air Pollution: Physical and Chemical Fundamentals</i>, McGraw-Hill, New York, 1975. 13. R. M. Harrison (Ed), <i>Pollution: Causes, Effects and Control</i>, Royal Society of Chemistry, Great Britain, 1990. 14. J. E. Fergusson, <i>The Heavy Elements: Chemistry, Environmental Impact and Health Effects</i>, Pergamon Press, Oxford, 1990. 15. A. K. De, <i>Environmental Chemistry</i>, 4th Edn, New Age International (P) Ltd. Publications, New Delhi, 2000. 16. D. F. S. Natusch and P. K. Hopke, <i>Analytical Aspects of Environmental Chemistry</i>, John Wiley and Sons, New York, 1983. 17. O. Hutzinger (Ed.), <i>The Handbook of Environmental Chemistry</i>, Springer-Verlag, Weinheim, 1980. 18. W. W. Wendlandt, <i>Thermal Methods of Analysis</i>, Interscience Publishers, New York, 1964. 19. D. Dollimore, <i>General Review on Thermal Analyses</i>, Anal. Chem., 1994, 66, 17R. 20. R. C. McKenzie (Ed.), <i>Differential Thermal Analysis</i>, Academic Press, New York, 1970. 21. C. Duval, <i>Inorganic Thermogravimetric Analysis</i>, Elsevier Publishing Co, New York, 1963. 22. D. R. Crow, <i>Polarography of Metal Complexes</i>, Academic Press, London, 1979. 23. C. G. Zoski (Ed) <i>Handbook of Electrochemistry</i>, Elsevier, New York, 2007 24. A. J. Bard and L. F. Faulkner, <i>Electrochemical Methods – Fundamentals and Applications</i>, 2nd Edn., Wiley, New York, 1998. 25. G. Seaborg, <i>Modern Alchemy</i>, World Scientific, 1994. 		
CHE-491	<p>Physical Chemistry Laboratory II</p> <ol style="list-style-type: none"> 1. To study Beer's law by spectrophotometric method of Iron-phenanthroline complex. 2. Determination of hydrodynamic volume of denatured protein. 3. Determination of particle size by Survisometer 4. Determination of adsorption capacity of activated charcoal 5. Experiments on kinetics-I: effect of solvent, pH, ionic strength 	3	2
CHE-492	<p>Inorganic Chemistry Laboratory II</p>	3	2

	<ol style="list-style-type: none"> 1. Electrical conductivity measurements, and spectral, thermal, electrochemical and magnetic studies of coordination compounds 2. Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric methods 3. Special identification tests for mixture of acid radicals; qualitative analysis of less common elements-Mo, W, Ti, Zr, Th, V, U (two metal ion in cationic/anionic forms). 4. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe using volumetric and gravimetric methods 5. Chromatographic separation: <ol style="list-style-type: none"> a. Cd and Zn b. Zn and Mg 		
CHE-493	Organic Chemistry Laboratory II <ol style="list-style-type: none"> 1. Different types of chromatography including low and medium pressure condition; purification techniques: vacuum distillation and sublimation, solvent purification, crystallization, 2. Chromatographic Separation <ol style="list-style-type: none"> a. Column Chromatography: separation of mixture of ortho and para-Nitroanilines. b. Thin Layer Chromatography: separation of mixture of ortho and para – Nitroanilines. c. Paper chromatography – identification of alpha amino acids. 3. Quantitative estimation of ascorbic acid 	3	2

SEMESTER- III

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-501	Inorganic Chemistry III <p>UNIT I <i>Metal ion promoted reactions:</i> Fundamentals, simple cycle, catalytic cycle, pliancy of substrates, oxidative addition, reductive elimination, insertion; Tolman catalytic loop, homogeneous/heterogeneous catalysis: Wacker-Smidt synthesis, hydroformylation reactions, Monsanto acetic acid process, hydrogenation by Wilkinson's catalyst, water gas shift reaction (WGSR), Fischer-Tropsch synthesis, alkene polymerization, hydrosilation, hydrophosphilylation, hydroamination, hydrocyanation and hydroboration reactions, Heck reaction</p> <p>UNIT II <i>Complexes in aqueous solution:</i> Different (pH-potentiometric, spectrophotometric, voltammetric) tools and methods (slope-ratio, mole-ratio and Job's method of continuous variation) of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; evaluation of thermodynamic parameters, factors influencing the stability of complexes, equilibria in biomolecular systems</p>	1	3

UNIT III

Reaction mechanism: Fundamentals, analysis of rate data, H⁺-terms in rate laws, complex rate laws, kinetically indistinguishable schemes, rate scale, mechanistic simulation; associative, dissociative, interchange, nucleophilic, electrophilic pathways; Hammett relation, linear free energy relationship

Molecular magnetism: Different magnetic materials, use of Pascal's constants in structure determination, van Vleck equation and its applications, Curie and Curie-Weiss laws, Lande interval rule, microstates, multiplet, multiplet width, hole formalism, zero-field splitting, spin-orbit coupling, quenching of orbital contribution, crystal field diagram, high spin/low spin equilibrium

Reference Books:

1. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
2. G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
3. G. Wulfsberg, *Principles of Descriptive Inorganic Chemistry*, University Science Books, Mill Valley, CA, 1991.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edn, Harper Collins College Publishers, New York, 1993. 24
5. G. B. Richter-Addo and P. L. Legzdins, *Metal Nitrosyls*, Oxford University Press, New York, 1992.
6. J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.
7. G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.
8. C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.
9. C. G. Zoski (Ed) *Handbook of Electrochemistry*, Elsevier, New York, 2007
10. A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications*, 2nd Edn., Wiley, New York, 1998.
11. R. M. Smith and A. F. Martell, *Critical Stability Constants*, 6 Vols, Plenum Press, New York, 1974-89.
12. A. E. Martell and R. J. Motekaitis, *Determination and use of Stability Constants*, 2nd Edn, VCH, New York, 1992.
13. M. Meloun, J. Havel and E. Hogfeldt, *Computation of Solution Equilibria: A Guide to Methods in Potentiometry, Extraction and Spectrophotometry*, Halsted, New York, 1988.
14. F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, 1967.
15. R. G. Wilkins, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
16. D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley and Sons, New York, 1987.
17. D. Benson, *Mechanism of Inorganic Reactions in Solution*, McGraw-Hill, London, 1968.
18. R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 1998.
19. J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.
20. C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.
21. O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
22. J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, II: Molecule-Based Magnets*, Wiley-VCH, Weinheim, 2001.
23. P. M. Lathi (Ed), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.

CHE-502	<p>Physical Chemistry III</p> <p>UNIT I <i>Group theory:</i> Application of group theoretical methods for (i) construction of SALC's and their use in calculation of π MO's under the Huckel approximations, (ii) calculation of MO's of AB_n type and sandwich type molecules, (iii) study of hybridization, selection rules, allowedness/forbiddenness of $n-\pi^*$ and $\pi-\pi^*$ transitions, (iv) splitting of terms in octahedral and tetrahedral ligand fields, Orgel and Tanabe-Sugano diagrams, (v) symmetry aspects of molecular vibrations – infrared and Raman activity, conservation of orbital symmetry in pericyclic reactions <i>Macromolecules:</i> Introduction; Carother's equation, osmotic pressure, viscosity, sedimentation and light scattering experiments for determination of molecular weight; kinetics of addition and condensation polymerization, stereochemistry, flexibility of polymer chain, statistics of polymer dimensions and configurations, effect of solvent on the average dimensions; theories of polymer solutions: excluded volume and Flory-Huggins theory</p> <p>UNIT II <i>Surface chemistry:</i> Introduction, adsorption, surface excess; BET isotherm, LB film, membrane equilibrium, micellisation, catalytic activity, surface active agent, Classification of surface active agent, Critical Micellar Concentration (CMC), Factor affecting the CMC of surfactants, hydrophobic interaction, thermodynamics of micellization-phase separation and mass action model, micro emulsion, reverse micelles. <i>Basic principles of catalysis:</i> Frenlich, Langmuir, BET, Gibb's adsorption isotherms, surface area, pore size and acid strength measurement. Thermodynamics of adsorption: interpretation of chemisorptions based on the structure and nature. Kinetic of surface reactions: rate determining step, various types of reaction, simple, parallel and consecutive reactions. Surface films on liquid (electrokinetic phenomenon)</p> <p>UNIT III <i>Advanced spectroscopic methods:</i> Instrumentation, presentation of spectra, active chemical system; INDOR, COSY, NOESY in ^1HNMR; functional group characterization, fluxionality, distortion and dynamic equilibria; long-range spin-spin interaction; ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{19}F and ^{31}P-NMR: instrumentation, chemical shift and application; EI, CI, FD, FAB-Mass, MALDI-TOF; isotropic effect, fragmentation patterns and application in structure elucidation; CD/ORD: methods, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application; EPR: anisotropy, intensity, hyperfine splitting, Kramer's theorem, photoelectron spectroscopy, ESCA, UPS, Auger, AES, XRF and EXFAS; Synergistic benefit: spectroscopic and other tools in structure elucidation</p> <p><u>Reference Books:</u> 1. F. A. Cotton, <i>Chemical Applications of Group Theory</i>, 3rd Edn Reprint, John</p>	1	3
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	<p>Wiley and Sons, New York, 1999.</p> <ol style="list-style-type: none"> 2. A. Vincent, <i>Molecular Symmetry and Group Theory</i>, John Wiley and Sons, New York, 1998. 3. S. C. Rakshit, <i>Molecular Symmetry Group and Chemistry</i>, The New Book Stall, Kolkata, 1988. 4. V. Heine, <i>Group Theory in Quantum Mechanics: An Introduction to Its Present Usage</i>, Dover Publication, New York, 1991. 5. W. Adamson, <i>Physical Chemistry of Surfaces</i>, John Wiley and Sons, New York, 1990 6. H. -J. Butt, K. Graf and M. Kappl, <i>Physics and Chemistry of Interfaces</i>, Wiley-VCH, 2003. 7. J. H. Clint, <i>Surface Chemistry</i>, Blackie and Son Ltd., 1992. 8. G. S. Mishra, <i>Introductory Polymer Chemistry</i>, Wiley Eastern, New Delhi, 1993. 9. G. W. Castellan, <i>Physical Chemistry</i>, 3rd Edn., Narosa Publishing House, 1995. 10. R. A. Alberty and R. J. Silbey, <i>Physical Chemistry</i>, 1st Edn., John Wiley and Sons, Inc., New York, 1995. 11. P. Ghosh, <i>Polymer Science and Technology of Plastic and Rubber</i>, Tata McGraw-Hill Publishing Company Limited, New Delhi, 1993. 12. C. Tanford, <i>Physical Chemistry of Macromolecules</i>, John Wiley and Sons, Inc., New York, 1961. 13. I. N. Levine, <i>Physical Chemistry</i>, 4th Edn., Tata McGraw-Hill, New Delhi, 1995. 22 14. S. F. Sun, <i>Physical Chemistry of Macromolecules: Basic Principles and Issues</i>, John Wiley & Sons, New York, 1994. 15. F. W. Billmeyer, <i>Text Book of Polymer Science</i>, 2nd Edn., Wiley-Interscience, New York, 1971. 16. C. N. Banwell and E. M. McCash, <i>Fundamentals of Molecular Spectroscopy</i>, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994. 17. R. S. Drago, <i>Physical Methods for Chemists</i>, Saunders, Philadelphia, 1992. 18. J. G. Grasselli, M. K. Snavely and B. J. Bulkin, <i>Chemical Application of Raman Spectroscopy</i>, Wiley, New York, 1981. 19. P. Hendra, C. Jones and G. Warnes, <i>FT-Raman Spectroscopy</i>, Ellis-Harwood, 1991. 20. K. Nakamoto, <i>Infrared and Raman Spectra of Inorganic and Coordination Compounds</i>, 5th Edn, Part B, John Wiley and Sons, Inc., New York, 1997. 21. W. Kemp, <i>NMR in Chemistry: A Multinuclear Approach</i>, Macmillan Press, 1986. 22. H. Gunther, <i>NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry</i>, Wiley, New York, 1995. 23. N. M. Atherton, <i>Principles of Electron Spin Resonance</i>, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993. 24. L. Kevan and R. N. Schwartz (Eds), <i>Time Domain Electron Spin Resonance</i>, John Wiley, New York, 1979. 25. J. E. Wertz and J. R. Boulton, <i>Electron Spin Resonance: Elementary Theory and Practical Applications</i>, Chapman and Hall, London, 1986. 26. D. W. Turner, C. Baker and C. R. Bundle, <i>Molecular Photoelectron Spectroscopy</i>, Wiley Interscience, New York, 1970. 27. J. H. D Eland, <i>Photoelectron Spectra</i>, Butterworth, London, 1984. 28. T. L. Barr, <i>Modern ESCA: the Principles and Practice of X-ray Photoelectron Spectroscopy</i>, CRC Press, Boca Raton, 1994. 29. D. P. Woodruff and T. A. Delchar, <i>Modern Techniques of Surface Science</i>, Cambridge University Press, Cambridge, 1988. 30. T. Thomson, M. D. Baker, A. Christie and J. F. Tyson, <i>Auger Electron Spectroscopy</i>, John Wiley, 1985. 		
CHE-503	<p>Organic Chemistry III</p> <p>UNIT I</p> <p><i>Photochemistry</i>: Photochemical energy, Jablonski diagram, Franck-Condon principle, photosensitisation and quenching, Norrish type-I and type-II processes, Paterno-Buchi reaction, photochemistry of</p>	1	3

unsaturated compounds: rearrangement of unsaturated compounds; photo-induced reactions in aromatic compounds, Principles and applications of photochemical reactions in organic chemistry.

Enzyme chemistry: Introduction, classification, formation and function of enzymes, co-enzymes, cofactors (elementary idea);

Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.

UNIT II

Pericyclic Reaction: Definition, classification, cyclo-additions and cyclo-reversion reactions, [2+2], [2+4], [4+6] reactions, catalysis; electrocyclic reaction and the electroreversion reactions; sigmatropic reactions of [i,j] and [j,j] types, regioselectivity, periselectivity in cycloadditions; generalised rules of pericyclic reactions, applications of *Pericyclic* reactions.

Reaction with cyclic transition states or cyclic intermediates: Tethering, Robinson annulations, iodolactonisation; synthesis of transfused ring; sulfur as a tether

UNIT III

Reagents in organic synthesis: Hydride transfer reagent/reduction: (i) Boranes, trialkylborohydrides, Diimide, Baker's yeast, trialkyl tin hydride, DIBAL, Na(CN)BH₃, NaBH₄, triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; LiAlH₄, and Red-Al; Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction (ii) Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata) (iii) enzymatic reduction

Oxidations: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium: PCC, PDC, Mn(IV) oxide, RuO₄ (TPAP)), (b) DMSO, hypervalent iodine (IBX, Moffat oxidation, Swern oxidation, Dess-Martin Periodinane) and TEMPO based reagents. (c) phenols (Fremy's salt, silver carbonate) (d) Wacker oxidation, (e) selenium, chromium based allylic oxidation, (f) Woodward and Prevost hydroxylation, (g) Sharpless epoxidation, (h) Shapiro reaction, (i) Peterson reaction, (j) OsO₄, (k) SeO₂ (l) enzymatic oxidation

Organic transformations: Functional group interconversion including oxidations and reductions; Chemo, regio and stereoselective transformations.

Reductions: Catalytic hydrogenation (Heterogeneous: Palladium/Rhodium/Nickel; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation.

Reference Books:

1. T.L.Gilchrist and R.C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn., Cambridge University Press, 1979.
2. R.B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, VerlagChemie GmbH, 1970.
3. T.H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn., Harper and Row, 1998.
4. A. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, John Wiley, 1980.
5. W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn., Low Price

	<p>Edition, Cambridge University Press, 1996.</p> <p>6. H. O. House, <i>Modern Synthetic Reactions</i>, 2nd Edn., Benjamin, 1971</p> <p>7. J. Singh and J. Singh, <i>Photochemistry and Pericyclic Reactions</i>, 2nd Edn., New Age International (P) Ltd., 2005</p>		
CHE-504	<p>Analytical Chemistry III</p> <p>UNIT-I <i>Electroanalytical Methods I:</i> Polarography and cyclic voltametry: Introduction, Instrumentation, Ilkovic equation and its verification. Derivation of wave equation, Determination of half wave potential, qualitative and quantitative applications. Amperometry: Basic principles, instrumentation, nature of titration curves, and analytical applications.</p> <p>UNIT-II <i>Complexometric titrations:</i> Stability of complexes, factors influencing the stability of complexes, stability constants of EDTA complexes, titration curves, selectivity, masking and demasking agents, metal ion indicators. Precipitation titrations: Theory of precipitation reactions, determination of endpoints in precipitation reactions, adsorption indicators.</p> <p>UNIT-III <i>Electroanalytical methods II:</i> Cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV; methods, choice of solvent, supporting electrolyte, working electrode, switching potential, electrode potential, pathways of electron transfer: EEE, ECE; electro-induced reactions; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn, ZEBRA system</p> <p>Reference Books:</p> <ol style="list-style-type: none"> 1. Analytical Chemistry: (J.W) G. D. Christain 2. Introduction to chromatography: Bobbit 3. Instrumental Methods of analysis (CBS)-H.H. Willard, L.L. Mirrit, J. A. Dean 4. Instrumental Methods of Analysis: Chatwal and Anand 5. Instrumental Methods of Inorganic Analysis (ELBS): A.I. Vogel 6. Chemical Instrumentation: A Systematic approach- H. A. Strobel 7. Principal of Instrumental Analysis-D. Skoog and D. West 	1	3
CHE-541	<p>Organic Chemistry Laboratory III</p> <ol style="list-style-type: none"> 1. Preparation of organic compounds involving multiple step reactions 2. Characterization of organic compounds using spectrophotometric methods 3. Separation and identification of sugars present in given mixture of glucose, fructose and sucrose by paper chromatography and determination of their R_f values. 	3	2
CHE-542	<p>Physical Chemistry Laboratory III</p> <ol style="list-style-type: none"> 1. Determination of partition coefficient in a biphasic system 2. Determination of density of upper and lower critical solution temperature (UCST/LCST) 3. IFT determination of immiscible solution 4. Determination of pK_a of an indicator. 5. Experiments on surface chemistry: determination of CMC by conductometric, tensiometric, viscometric and spectrophotometric methods 6. Experiments on kinetics-II: variable temperature, 	3	2

	experiments on equilibrium, micelles		
CHE-543	Inorganic Chemistry Laboratory III <ol style="list-style-type: none"> Preparation of inorganic and coordination compounds and characterization <ol style="list-style-type: none"> Bi-, tri-, and polydentate ligands Complexation and purification Growing of single crystals Spectral, thermal, electrochemical Kinetic and mechanistic studies of some selected reactions (substitution and redox) Volumetric analysis: redox, complexometric and precipitation titrations. Reaction of Cr(III) with a multidentate ligand: a kinetic experiment (Visible spectra Cr-EDTA complex) Preparation copper glycine complex cis- and trans- bis (glycinato Copper (II)) 	3	2

SEMESTER- IV

<i>COURSE NO.</i>	<i>COURSE TITLE</i>	<i>COURSE CODE</i>	<i>CREDIT</i>
CHE-551	Inorganic Chemistry IV <p>UNIT I <i>Synthetic methodology for transition and non-transition metal compounds:</i> Ligand design and ligand synthesis: polypyridine, Schiff base, oxime, macrocycle, tripod, podand, coronand, cryptand, octopus, tailoring and appending of pendant arm, electron reservoir, ligand topology and molecular mechanics, coordination compound design and synthesis: self-assembly, structure-directed synthesis, building block, metalloligand, polymeric ensembles (chain, sheet, network), supramolecular framework, molecular machine, biomodelling, molecular/crystal engineering</p> <p>UNIT II <i>Inorganic reaction mechanism I:</i> Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, inorganic nucleophilicity scales; Edward scale, n_{pt} scale, Gutmann donor number, Drago E & C scale, trans effect, cis effect, reactions without metal-ligand bond breaking, water exchange rates, proton ambiguity, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions.</p> <p>UNIT III <i>Inorganic reaction mechanism II:</i> Kinetic and activation parameters: a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand; reactions in fluxional organometallic compounds</p>	1	3

Reference Books:

1. L. S. Hegedus, *Transition Metal in the Synthesis of Complex Organic Molecules*, University Science Press, Mill Valley, CA, 1994.
2. M. Periasamy, *Organic Synthesis Using Iron-Carbonyl Reagents*, *Curr. Sci.*, 2000, 78, (11), 1307-1313
3. G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
4. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
5. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn, Pergamon, New York, 1997.
6. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.
7. G. R. Desiraju, *Crystal Engineering: Designing of Organic Solids*, Elsevier, New York, 1989.
8. F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, 1967.
9. R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
10. D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley and Sons, New York, 1987.
11. D. Benson, *Mechanism of Inorganic Reactions in Solution*, McGraw-Hill, London, 1968.
12. R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 1998.
13. J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.
14. C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.
15. G. Aruldas, *Molecular Structure and Spectroscopy*, 2nd Edn., Prentice-Hall of India, New Delhi, 2007.
16. D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University press, 2001.
17. R. S. Drago, *Physical Methods in Inorganic chemistry*, Saunders, Philadelphia, 1977.
18. C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
19. A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.
20. D. N. Sathyanarayana, *Vibrational Spectroscopy Theory and Applications*, New Age International, New Delhi, 1996.
21. H. H. Jaffe and M. Orchin, *Symmetry, Orbitals and Spectra*, Wiley, New York, 1982.
22. B. E. Douglas and C. A. Hollingsworth, *Symmetry in Bonding and Spectra, An Introduction*, Academic press, New York, 1985.
23. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 5th Edn, Part A, Wiley, New York, 1997.
24. B. Schrader (Ed.) *Infrared and Raman Spectroscopy: Methods and Applications*, VCH Weinheim, 1995.
25. W. Henderson and J. S. McIndoe, *Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools-Techniques-Tips*, John Wiley & Sons, Ltd., Chichester, 2005.
26. A. E. Derome, *Modern NMR Techniques in Chemical Research*, Pergamon Press, Oxford, 1987.
27. W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, 1986. 28
28. J. K. M. Sanders, E. C. Constable and B. K. Hunter, *Modern NMR Spectroscopy: A Workbook of Chemical Problems*, Oxford University Press, Oxford, 1993.
29. H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.
30. A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal Ions*, Clarendon Press, Oxford, 1970.
31. N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.

	<p>32. W. O. George and H. O. Willis, <i>Computer Methods in Ultraviolet, Visible and Infra-red Spectroscopy</i>, Royal Society of Chemistry, 1990.</p> <p>33. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, <i>Structural Methods in Inorganic Chemistry</i>, 2nd Edn., Blackwell Scientific Publications, Oxford, 1991.</p> <p>34. F. Gerson, <i>High Resolution ESR. Spectroscopy</i>, John Wiley, New York, 1971.</p> <p>35. L. Kevan and R. N. Schwartz (Eds), <i>Time Domain Electron Spin Resonance</i>, John Wiley, New York, 1979.</p> <p>36. J. E. Wertz and J. R. Boulton, <i>Electron Spin Resonance: Elementary Theory and Practical Applications</i>, Chapman and Hall, London, 1986.</p>		
CHE-552	<p>Physical Chemistry IV</p> <p>UNIT I <i>Thermodynamics of irreversible processes:</i> Limitations of classical thermodynamics, entropy change in irreversible processes, concept of forces and fluxes, linear phenomenological relations; Onsager reciprocity relation – derivation from fluctuation theory; Curie-Prigogine principle – statement and proof using one scalar and one vector force, illustrations; Saxen’s relations in connection with electrokinetic phenomena and their proof using Onsager reciprocity relations, stationary states: variation of entropy change with time, Prigogine’s criterion for establishment of stationary state, applicability of Le Chatelier’s principle on stationary states</p> <p>UNIT II <i>Chemical Kinetics:</i> Introduction, autocatalysis, chain reactions: branched and non-branched kinetic rate equations, Semenov treatment for branched chain reactions; explosion: population explosion, upper and lower ignition and explosion limits; thermal ignition and ignition temperature; oscillator reaction: Lotka, Oregonator and Brusselator; conditions for oscillation, chemistry of BZ reaction (Brusselator model); theories of unimolecular reactions: Lindemann, Hinshelwood and RRK theory</p> <p>UNIT III <i>Non-ideal systems:</i> Virial equations, fugacity and standard state; gas mixtures, partition function of non-ideal gas, derivation of non-ideal equation of state, second Virial coefficient; existence of Boyle and inversion temperature for real gases, derivation of Van der Waals equation, thermodynamic functions of real gases; non-ideal solutions; activity and activity coefficients; different scales; methods of their determinations; partial molar quantities and their determinations, Duhem-Margules equation and its applications, regular solutions and excess thermodynamic functions <i>Photochemistry:</i> Generation of excited states, singlet and triplet states, spin-orbit coupling, radiative and non-radiative processes, fluorescence and phosphorescence: mirror image relationship, quantum yield, life-time and anisotropy; properties of excited states: dipole moment, pK_a, energy transfer, quenching, excimers and exciplexes, special photochemical reactions, flash photolysis, laser flash photolysis</p> <p>Reference Books:</p> <ol style="list-style-type: none"> 1. I. Prigogine, <i>Introduction to Thermodynamics of Irreversible Processes</i>, Interscience Publishers, 1967. 2. V. N. Kondrat’ev, <i>Chemical Kinetics of Gas Reactions</i>, Pergamon Press, 1964. 	1	3

	<ol style="list-style-type: none"> 3. P. C. Jordan, <i>Chemical Kinetics and Transport</i>, John Wiley and Sons, Inc., 1979. 4. M. J. Pilling and P. W. Seakins, <i>Reaction Kinetics</i>, Oxford University Press, 1995. 5. M. R. Wright, <i>Fundamental Chemical Kinetics</i>, Horwood Publishing, 1999. 6. S. K. Scott, <i>Oscillations, Waves, and Chaos in Chemical Kinetics</i>, Oxford University Press, 1994. 7. E. N. Yeregin, <i>The Foundation of Chemical Kinetics</i>, Mir Publishers, 1979. 8. K. J. Laidler, <i>Chemical Kinetics</i>, TMH Publishing Company Limited, 1988. 9. E. Kreyszig, <i>Advanced Engineering Mathematics</i>, 5th Edn., Wiley Eastern, 1988. 10. G. Arfken, <i>Mathematical Methods for Physicists</i>, Academic Press, New York, 1966. 11. M. K. Jain, <i>Numerical Methods for Scientific and Engineering Computation</i>, Wiley Eastern Ltd. 12. R. A. McQuarrie and J. D. Simons, <i>Physical Chemistry</i> 1st Edn, Viva Books Private Limited, New Delhi, 1998. 13. R. A. McQuarrie, <i>Statistical Mechanics</i>, Harper and Row, 1976. 14. L. D. Landall and E. M. Lifshitz, <i>Statistical Physics</i> 2nd revised English Edn., Pergamon Press, Oxford, 1977. 15. J. N. Murrell, <i>The Theory of Electronic Spectra of Organic Molecules</i>, John Wiley and Sons, 1963. 16. J. B. Burks, <i>Photophysics of Aromatic Molecules</i>, Wiley-Interscience, 1969. 17. G. M. Burnett and A. M. North, <i>Transfer and Storage of Energy by Molecule</i>, Vol. I, Wiley-Interscience, 1970. 		
CHE-553	<p>Organic Chemistry IV</p> <p>UNIT I <i>Organometallic chemistry:</i> Bonding in transition metal; organometallic complexes; some common properties of organometallic complexes; fluxionality, stabilisation of reactive or unstable molecules; catalytic hydrogenation, insertion reactions; organo-Cu, -Zn, -Cd, -Hg and -Pd compounds; metallocenes (Fe, Ru, Os); carbene and carbyne complexes <i>Stereo selective reactions of alkenes and carbonyl compounds:</i> Nucleophilic addition: use of chiral substrates, auxiliaries, reagents and catalysts; asymmetric conjugate addition; addition of allyl boron derivative; reactions at alpha carbon: enolate formation (regioselectivity and stereoselectivity); stereoselective enolate alkylation (oxazolidinone, oxazoline); aldol reaction, asymmetric aldol reaction; hydroboration, hydrogenation, dihydroxylation, cyclopropanation, epoxidation <i>ORD-CD:</i> Introduction, theory, cotton effect curves and applications, octant rule, axial haloketo rule, lactone sector rule</p> <p>UNIT II <i>Terpenes:</i> Structural studies on sesquiterpenes, diterpenes, triterpenes and carotenoids; chemistry of carryophyllene, abietic acid, β-amyrin, α and β-carotenoids <i>Nucleic acids:</i> Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of nucleic acid. Structure, stereochemistry, synthesis and biosynthesis <i>Alkaloids:</i> Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and</p>	1	3

biosynthesis of the following: Papaverine, Ephedrine, Nicotine, Atropine, Quinine, Noscapine and Morphine.

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone. Biosynthesis of steroids

Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE₂ and PGF_{2a}.

UNIT III

¹³C NMR spectrometry: Introduction, theory, instrumentation, chemical shifts, coupling constants, application in organic molecule characterization

2D, 3D and other advanced NMR: Introduction, theory, instrumentation, chemical shifts, coupling constants, application in organic molecule characterization

Green Chemistry: Introduction: Prospects and future of Green Chemistry, Twelve guiding principles of green chemistry.

Approaches for green synthesis/reaction: Green starting materials, Green reagents, Green solvents and reaction conditions, Green catalysis, Green synthesis- Real world cases (Traditional Vs. Green processes) Synthesis of Ibuprofen, Adipic acid

Future trends in Green Chemistry: Biomimetic, multifunctional reagents; Combinatorial green chemistry; Non-covalent derivatization, Biomass conversion, emission control. Bio-catalysis.

Green Solvents:

- a. Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability
- b. Ionic liquids
- c. Supercritical fluids
- d. Solvent free neat reactions in liquid phase
- e. Solvent free neat reactions
- f. Fluorous phase reactions

Non-Conventional Energy Sources: Microwave and Ultrasound assisted reactions, photochemical reactions using sunlight

Green Catalysis: Heterogeneous catalysis: Use of zeolites, silica, alumina, clay, polymers, cyclodextrins, and supported catalysts. Biocatalysis: enzymes, microbes, Phase-transfer catalysis (micellar/surfactant)

Reference Books:

1. T.H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn., Harper and Row, 1998.
2. J. March, *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 5th Edn., John Wiley, 1999.
3. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4th Edn., Plenum Press, 2001.
4. K.C. Nicolson and E.J. Sorensen, *Classics in Total Synthesis*, VCH, 1996.
5. P. Deslongchamps, *Stereoelectronic Effect in Organic Chemistry*, Pergamon Press, 1983.
6. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd Edn., ELBS, 2003..
7. W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn., Low Price Edition, Cambridge University Press, 1996. 31
8. S. Hanessain, *Total Synthesis of Natural Products : The Chiron Approach*, Pergamon Press, 1984.

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CHE-554	<p>Analytical Chemistry IV</p> <p>UNIT I</p> <p>Gravimetric Methods of Analysis: Gravimetric methods, Calculation of results from gravimetric data, Properties of precipitates and precipitating reagents, Size of precipitate particles, Factors affecting particle size; Characteristics of precipitation reactions: variables that</p>	1	3

	<p>minimize supersaturation, improving filterability, co-precipitation, drying precipitates; Critique of gravimetric methods: time, equipment' sensitivity and accuracy, specificity</p> <p>UNIT II <i>Instrumental techniques in chemical analysis:</i> Introduction, Theory, Instruments, working and Applications Radiochemical Analysis, NAA: Scintillation counter and G.M. Counter, Atomic Absorption Spectroscopy Introduction, Principal, advantages and disadvantages of AAS and AES. Instrumentation, Single and double beam AAS, detection limit and sensitivity, Interferences applications.</p> <p>UNIT III Working principal and application of EDX, SEM, TEM, pXRD, HPLC, GC, FT-NMR, FT-Mass, TG-DTA, DSC, QESL/DLS, AFM, Nephelometry and Turbidometry, BET, Rheometer, Polarimeter, CV, ORD, Zeta potential, DLS, Survisometer; Inductively coupled Plasma Spectroscopy, Nebulisation Torch, Plasma, Instrumentation, Interferences</p> <p>Reference Books:</p> <ol style="list-style-type: none"> 1. Instrumental Methods of analysis- Willard, Merrit, Dean and Settle. 2. Spectroscopic identification of organic compounds- R.M. Silverstein and G. C. Bassler 3. Spectroscopic methods in organic chemistry- D.H. Williams and I. Fleming 4. Absorption spectroscopy of organic molecules- V.M. Parikh 5. Applications of spectroscopic techniques in Organic chemistry- P.S. Kalsi 6. A Text book of Qualitative Inorganic Analysis- A. I. Vogel 7. Physical Methods in Inorganic Chemistry (DWAP)- R. Drago 8. Fundamentals of Analytical Chemistry – D.A. Skoog and D.M. West (Holt Rinehart and Winston Inc). 		
CHE-591	<p>Organic Chemistry Laboratory IV</p> <ol style="list-style-type: none"> 1. Green oxidation reaction for Synthesis of adipic acid 2. Solvent free reaction (Microwave-assisted ammonium formate-mediated Knoevenagel reaction) 3. Green photochemical reactions Photoreduction of benzophenone to benzopinacol 4. Extraction of Natural Products: <ol style="list-style-type: none"> a. Caffeine from tea leaves. b. Citric acid from lemon. c. Lactose and casein from milk 	3	1
CHE-592	<p>Physical Chemistry Laboratory IV</p> <ol style="list-style-type: none"> 1. Determination of stability colloidal solution using friccohesity 2. To determine adulteration in dairy product, Ink and petrol. 3. Determination osmotic pressure, conduction, surface tension, viscosity of a solution together by Oscosurvismeter. 4. Preparation of buffer solutions and determination of their pH values. 5. Potentiometric titration of phosphoric acid using NaOH and standard Potassium hydrogen phthalate. 6. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte. 	3	1
CHE-593	<p>Inorganic Chemistry Laboratory IV</p>	3	1

	<ol style="list-style-type: none"> 1. Spectrophotometric determinations of metals <ol style="list-style-type: none"> a) Manganese/Chromium/ Vanadium in steel sample. b) Nickel/ Molybdenum/ Tungsten by extractive spectrophotometric method c) Fluoride/ nitrite/ phosphate d) Zirconium-Alizarin Red-S complex-Mole ration method e) Copper ethylene diamine complex: Slope-ratio method 2. Flame photometric determinations <ol style="list-style-type: none"> a) Sodium and potassium in blood serum b) Ca and Li in tap water 		
CHE-594	Project	3	3

PROJECT

A student is free to pick up a topic for the project at the beginning of Semester III. The student is expected to complete the major literature survey during the Semester III and present a tentative research plan at the end of Semester III. The candidate will do the experimental work during Semester IV under the supervision of a guide and submit the results in the form of a thesis at the end of Semester IV. The project will be evaluated by the concerned guide.