CENTRAL UNIVERSITY OF RAJASTHAN

M.Sc. (CHEMISTRY) PROGRAMME

1. PREAMBLE

The purpose of post-graduate education in Science is to create highly skilled manpower in specific areas, which will lead to generation of new knowledge and creation of wealth for the country. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of human beings by providing many of human requirements and essentialities. Chemistry is important to the world economy as well. The developments in Chemistry during last few decades are phenomenal. It is also seen that these developments are crossing the traditional vertical boundaries of scientific disciplines; the more inclination is seen towards biological sciences. New branches of chemistry are emerging and gaining importance, such as bioorganic chemistry, materials chemistry, computational chemistry, etc. The practice of Chemistry at industrial scale also is undergoing radical changes and is more or more based on deep understanding the chemical phenomena. The emerging Chemical Technologies are highly science based. The aid of computers has not only accelerated growth in the practice of Chemistry, but revolutionized the entire field. A Chemist cannot isolate himself from other disciplines. Thus, after a long span of more and more specialization in graduate and post-graduate syllabi, a symbiotic interdisciplinary approach now seems to be more relevant.

The practice of Chemistry, as is witnessed, over a span of more than a century has also created concomitant and perhaps unavoidable impacts of human environment. The adverse effects were particularly noted during last few decades. The concept of sustainable development is now well accepted. Though not a separate branch of Chemistry, Green Chemistry has emerged as a new approach to the practice of Chemistry on the background of sustainability. The Chemical Industry is now pressurized from both the Government and the Society to develop ecofriendly processes and products which will reduce waste and prevent toxic substances from entering the environment. The principles and applications of Chemistry should be learnt on this background.

2. OBJECTIVES

(i) To impart training in Chemistry at advanced level in a more wholistic way and enthuse the students for the subject;
(ii) To train the students to make them confident and capable of accepting any challenge in Chemistry,
(iii) To give a flavour of research in Chemistry and train the students for research career,

(iv) To abreast the students about the current status and new developments in Chemistry,
(v) To make the students aware of the impact of Chemistry on environment and imbibe the concept of sustainable developments,
(vi) To educate the students with respect to skills and knowledge to practice chemistry in ways that are benign to health and environment,
(vii) To provide flexibility in selecting some of the courses as per the interest and also to provide space for fast learners,
(viii) To make the students aware of resources and make them capable of mining the data.

3. DURATION OF THE PROGRAMME: Four semesters of two years

4. ADMISSION PROCEDURE:

The admission to the course shall be through an entrance examination to be conducted on all-India basis.

5. ELIGIBILITY OF THE CANDIDATES:

Candidates who have passed B.Sc. examination of any recognized university or its equivalent examination with minimum of 55% marks in aggregate (50% in the case of SC/ST students) and who have taken Chemistry as one of the subjects at the third year of the B.Sc.

6. SYLLABUS OF THE ENTRANCE EXAMINATION

The syllabus of the entrance examination is as declared by the University and put up on the website.

7. SEMESTERWISE STRUCTURE OF THE M.Sc. (CHEMISTRY) PROGRAMME

SEMESTER I

Code	Title of Course	Type of course	Level	h/week	Credits
CHT 101	Analytical Chemistry	Core	A	3	3
CHT 102	Chemistry of Main Group Elements	Core	A	3	3
CHT 103	Stereochemistry and Reaction Mechanism	Core	A	3	3
CHT 104	Electrochemistry and Kinetics	Core	A	3	3
CHT 105	Thermodynamics	Core	C	2	2
CHT 106	Communication Skills	Supportive	C	2	2
CHT 107	Mathematics for Chemists/ Biology for Chemists	Supportive	B	2	2
	Seminar				Audit

Practicals

CHP 101	Inorganic Chemistry Laboratory I		4	2	
CHP 102	Organic Chemistry Laboratory I		4	2	
CHP 103	Physical Chemistry Laboratory I		4	2	
	Safety			Audit	

SEMESTER- II

Code	Title of Course	Type	Level	h/week	Credits
CHT 201	Chemistry of Transition Metals	Core	A	3	3
CHT 202	Photochemistry, Pericyclic reactions, and Heterocycles	Core	A	3	3
CHT 203	Quantum Chemistry	Core	A	3	3
CHT 204	Organometallic Chemistry	Core	A	3	3
CHT 205	Organic Synthesis I	Core	A	3	3
CHT 206	Group Theory and Spectroscopy	Core	A	3	3
CHT 207	**Seminar**				Audit

Practicals

CHP 201	Inorganic Chemistry Laboratory II			4	2
CHP 202	Organic Chemistry Laboratory II			4	2
CHP 203	Physical Chemistry Laboratory II			4	2

SEMESTER- III

Code	Title of Course	Type	Level	h/week	Credits
CHT 301	Spectroscopy	Core	A	3	3
CHT 302	Organic Synthesis II	Core	A	3	3
CHT 303	Biomolecular Chemistry	Core	B	3	3
CHT 304	Environmental Chemistry	Supportive	B	2	2
CHT 305	Green Chemistry I	Core	B	3	3
CHT 306	Elective I	Core	A	2	2
CHT 307	Elective II	Supportive	C	2	2
CHT 308	**Project preparation**				Audit

Practicals

CHP 301	Inorganic Chemistry Laboratory III			4	2
CHP 302	Organic Chemistry Laboratory III			4	2
CHP 303	Physical Chemistry Laboratory III			4	2

SEMESTER- IV

Code	Title of Course	Type	Level	h/week	Credits
CHT 401	Green Chemistry II	Core	A	3	3
CHT 402	Solid state, Surfaces, & Catalysis	Core	A	3	3
CHT 403	Elective III	Core	A	2	2
CHT 404	Elective IV	Core	A	2	2
CHT 405	Elective V	Core	A	2	2
CHT 406	Elective VI	Supportive	A	2	2
CHP 401	**Project**				10

*** Project will be in the specialization area.**

8. DETAIL SYLLABUS

SEMESTER I

CHT 101 ANALYTICAL CHEMISTRY 3 CREDITS

UNIT I

1. Measurement and data analysis: Accuracy, precision, sensitivity and specificity. Significant figures. Determinate and indeterminate errors and minimization of errors, Gaussian distribution of data, standard deviation. Criteria for rejection of data-Q-test, Student t-test, F-test, Chi square test, confidence limit, control chart. Regression analysis, least squares method, correlation coefficient. **8L**

2. Solvent extraction: Classification, distribution law, separation factor, extraction equilibria and extraction systems - Chelation, solvation and ion-pair formation. Application in metal ion separation. Batch, continuous and counter current extractions. Membrane separation. **7L**

UNIT II

3. Chromatography: Types. Ion exchange chromatography, planar chromatography - paper and TLC. Stationary and mobile phases. GC – Theory, instrumentation and applications. Liquid-liquid partition chromatography. HPLC. Reverse phase chromatography. Size exclusion and Affinity chromatography. **9L**

4. Spectral methods: Basic Principles, Bear-Lambert Law. UV-Visible spectrophotometry -Instrumentation and application. AAS - Hollow cathode lamp, graphite furnace, interferences. AES. Flame photometry, ICP - AES. Fluorescence spectrophotometry - Principle and instrumentation. **6L**

UNIT III

5. Radioanalytical methods: Radioactivity as analytical tool. Neutron activation analysis - Instrumentation and application for trace and ultra trace analysis, isotope dilution analysis. **5h**

6. Thermal methods: TGA, DTA, DSC – Basics, instrumentation and applications. **3h**

7. Electroanalytical techniques: Polarography, conductometry, potentiometry, and coulometry, anodic stripping, Electrophoresis and its applications. **7L**

Reference Books:

1. Analytical Chemistry, Christian G.D., John Wiley & Sons Inc. 2004.
2. Fundamentals of analytical Chemistry. Skoog. D.A. West D.M. and Hooler F.J., W.B. Saunders.
3. Analytical Chemistry-Principles. Kennedy. J.H., W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques, LG. Hargis. Prentice Hall.
5. Principles of Instrumental Analysis by D.A. Skoog, Holler F.J. and Nieman T.A., 5^{th} Edn, Thomson Brooks/Cole, Bangalor, 2004.
6. Principles of Instrumental analysis Skoog D.A. and Loary J.L., Saunders W.B..
7. Quantitative Analysis, Day R.A., Jr. and Underwood A.L., Prentice Hall.
8. Basic Concepts of Analysis Chemistry, Khopkar S.M., Wiley Eastern.

9. Vogel's Textbook of Quantitative Chemical Analysis, by Menham J., Denney R.C., Barnes J.D. and Thomas M.J.K., 6th Edn, Low Price Edn, Pearson Education Ltd, New Delhi, 2000.
10. Instrumental Analysis, Editors, Christian G.D. and Reilly J.E. O', 2nd Edn, Allyn and Bacon, Inc., Boston,1986.
11. Principles and Practice of Analytical Chemistry by. Fifield F.W and Kealey D., 5th Edn, Blackwell Science Ltd, New Delhi, 2004.
12. Handbook of Instrumental Techniques for Analytical Chemistry, Editor, Settle F., Low Price Edn, Pearson Education Inc, New Delhi, 2004.
13. Instrumental Methods of Chemical Analysis by Ewing G.W., 5th Edn, McGraw Hill Singapore,1985.
14. Instrumental Methods of Analysis by Willard H.H., Merritt l.L., Dean J. A. & Settle F. A., CBS Publishers & Distributors, New Delhi, 1986.

CHT 102 CHEMISTRY OF MAIN GROUP ELEMENTS 3 CREDITS

UNIT I

1. Stereochemistry and Bonding in main group compounds: VSEPRT. Walsh diagram. Hybridization including energetics of hybridization. Bents rule, dπ-pπ bond. Some simple reactions of covalently bonded molecules (i) Atomic inversion (ii) Bery pseudo rotation (iii) Nucleophilic displacement (iv) Free radical mechanism **9L**

2. Hydrogen, alkali and alkaline earth metals: Classification of hydrides - e-deficient, e-precise & e-rich hydrides. Application of crown ethers in extraction of alkali and alkaline earth metals. **3L**

3. Noble gases: Isolation and properties. Preparation and structure of noble gas compounds **3L**

UNIT II

4. Boron compounds: Preparation, structure, bonding, reactions and applications of boranes, carboranes, metalloboranes, metallocarboranes, borazines. **6L**

5. Compounds of carbon and silicon: Fullerenes and their compounds, Intercalation compounds of graphite, carbon nano-tubes: Synthesis, structure, properties, and applications. Carbides, fluorocarbons, silanes, silicates, zeolites and silicones. **6L**

6. Compounds of oxygen group elements: Metal selenides and tellurides, oxyacids and oxoanions of S & N. **3L**

UNIT III

7. Compounds of nitrogen group elements: Nitrogen activation. Oxidation states of nitrogen and their interconversion. BN, PN and SN compounds - preparation, structure and bonding.

6L

8. Compounds of halogen group elements: Synthesis, properties, bonding, and applications of interhalogens, pseudohalogens, polyhalides, oxyacids and oxoanions of halogens **6L**

9. Reaction in non-aqueous solvents: Classification of solvents. Characteristic properties of an ionizing solvent. Reaction in liquid ammonia, liquid sulphur dioxide,

dimethyl formamide (DMF), dimethyl sulphoxide (DMSO) and dioxane. Chemistry of fused salt systems. **3L**

Reference Books:

1. Advanced Inorganic Chemistry, Cotton F.A. and Wilkinson G, John Wiley.
2. Inorganic Chemistry, Huhey J.E., Harper & Row.
3. Chemistry of the Elements, Greenwood N.N. and Earnshow A., Pergamon.
4. Inorganic Chemistry: A unified Approach, Porterfiels W. W., Elsevier
5. Inorganic Chemistry, Sharpe Alan G., Pearson Education Ltd.
6. Inorganic Chemistry, Shriver D.F., Atkins, P.W. and Langford C.H., Oxford University Press, 1998
7. Inorganic Chemistry, Miessler G. L. and Tarr D. A., Pearson Publications.
8. Inorganic Chemistry, Wulfsberg, G, University Science Books, Viva Books.

CHT 103 STEREOCHEMISTRY AND REACTION MECHANISM 3 CREDITS

UNIT I

1. Stereochemistry: 15L

1.1 Chirality: Stereogenic unit: Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of - allenes, spirans, biphenyls, cyclophanes, ansa compounds, *trans*-cyclooctene, helicenes, benzphenanthrenes. Configurational nomenclature.

1.2 Topicity and Prochirality: Topicity of ligands and faces. Diastereotopic ligands and NMR spectroscopy. Chemical reactivity of heterotropic ligands and faces with chiral and achiral reagents. Resolution of racemates.

1.3 Stereoselectivity and stereospecificity: Kinetic and thermodynamic controls, asymmetric induction, chiral auxilliary, diastereotopic induction, Cram's rule, Felkin's model, Prelog's rule.

1.4. Analytical methods: NMR: Chiral derivatising agents, chiral shift reagents, chiral solvating agents, chiral chromatography.

1.5 Conformational analysis of cycloalkanes: Cyclohexane, monosubstituted cyclohexanes, disubstituted cyclohexanes, effect of conformation on reactivity. Decalins. Conformational analysis of sugars. Anomeric effect. Strain due to unavoidable crowding.

1.6. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.

UNIT II

2. Reaction Mechanism: 15L

2.1 Structure and reactivity:

(a) Ambident electrophiles and nucleophiles; Hard and soft concept.
(b) Acidity and basicity: Different concepts. Controlling structural factors.
(c) Methods of determining reaction mechanism: Kinetic and non-kinetic methods. Hammet and Taft equations.

2.2 Nucleophilic substitution reactions:
(a) Recapitulation of S_N1, S_N2 ,S_N^i reactions with stereochemistry. S_NcA and S_N' reactions
(b) Nucleophilic substitutions at sp^2 hybridized carbon and aromatic ring, including vicarious substitution. Factors affecting reactivity.

2.3 Elimination reactions:
(a) E1, E2 and E1cB mechanisms. Orientation in elimination reactions.
(b) Reactivity: Effect of substrate, base, leaving group, medium. Pyrolytic elimination reactions.

2.5 Addition to carbon–carbon multiple bonds
Additions involving electrophiles and free radicals: Mechanism, reactivity, orientation and stereochemistry, regio- and chemo-selectivity.

UNIT III

2.4 Reactive intermediates: 5L
(a) Nonclassical carbocations. Neighbouring group participation.
(b) Carbenes, nitrenes, arynes – Generation, structure, reactions.

3. Radicals in organic synthesis 10L
(a) General aspects: Electrophilic and nucleophilic radicals and their reactivity with π-rich/deficient olefins.
(b) Inter- and intramolecular aliphatic C-C bond formation via mercury hydride, tin hydride, carbon hydride, thio donor (Barton's reaction).
(c) Cleavage of C-X, C-Sn, C-Co and C-S bonds in the generation of radicals.
(d) Trapping by electron transfer reactions using $Mn(OAc)_3$.
(e) Radical - Radical processes - oxidative couplings, single electron oxidation of carbanions to generate radicals, dehydrodimerization and Reductive couplings.
(f) C-C bond formation in aromatics - Introduction, radical reactions on aromatics, electrophilic radical reactions, nucleophilic radicals; Radical reactions on heteroaromatics- alkylation and acylations.

Reference Books

1. Organic stereochemistry, Robinson M.J. T., Oxford University Press, 2005.
2. Stereochemistry of Carbon compounds, Eliel E. L., Wilen S. H. and Manden L. N., Wiley, 1995.
3. Stereochemistry: Conformation & Mechanism, Kalsi P. S., Wiley Eastern Ltd., New Delhi, 1993.
4. Stereochemistry of Organic compounds, Nasipuri D., Wiley Eastern, 1991.
5. Advanced Organic Chemistry, Carey F.A. and Sundberg R.J., Plenum
6. A Guide book to mechanism in Organic chemistry, Sykes Peter, Prentice Hall.
7. Organic reaction mechanism (Benjamin) Breslow R.
8. Advanced Organic Chemistry: Reactions, Mechanism, and Structure, Smith M. B. and March J., John Wiley.
9. Reactive Intermediates in Organic chemistry Issacs N. S, John Wiley.
10. Organic Reaction Mechanisms: Ahluwalia V. K., Parashar R. K.
11. Reaction mechanism in Organic Chemistry, Mukherji S.M. and Singh S.P., Mcmillan.

12. Understanding Organic Reaction Mechanisms, Adam Jacobs, Cambridge University Press.
13. Advanced organic chemistry: Reaction mechanism, Reinhard Bruckener, Elsevier, 2008.
14. Advanced organic chemistry: Reactions and mechanism, M.S. Singh, Pearson Education, 2007
15. Why Chemical Reactions Happen (Paperback), by Keeler J. and Wothers P., Oxford University Press, 2003.

CHT 104 ELECTROCHEMISTRY AND KINETICS 3 CREDITS

UNIT I

1. Electrochemistry **15L**

1.1 Metal/Electrolyte interface: Genesis of double layer, potential profile across double layer region, polarizable and non-polarizable interfaces. Electrocapillary thermodynamics, surface excess quantities from electro capillary and capacitance measurement. Structure of the double layer: HB, GC, Stern and BDM models.

1.2 Fundamental of electrolytic corrosion: theories and kinetics, corrosion prevention. Batteries, fuel cells and electro catalysis.

1.3 Linear sweep voltametry. Cyclic voltametry, Charactersitcs of irreversible & reversible CV. Impedance measurements. AC voltametry.

UNIT II

2. Kinetics

2.1 Methods for determining reaction mechanism and rate laws. **5L**

2.2 Composite reactions - rate equation, steady state treatment. Fast reactions. oscillatory reactions. Autocatalysis. Flow techniques. Kinetic equations of flow systems, Relaxation techniques for different order reactions. Mechanism of atom and radical combination reactions. Flash photolysis - Shock tubes. **10L**

UNIT III

2.3 Enzyme catalyzed reactions: Kinetics of surface reactions and micellar catalysis. **3L**

2.4. Polymerization reactions: Condensation polymerization. Free radical and ionic polymerizations. Copolymerization reaction. **3L**

2.5 Reaction surface and dynamics: Potential energy surface, reaction coordinates and paths, transition state theory. Absolute rate theory, collision theory, reactions in solution. Statistical approach to rate theory: Hinselwood, RRK and RRKM theories. Molecular beam techniques. **9L**

Reference Books

1. Principles of electrochemistry, Koryta J., Dvorak J. and Kavan, L, John Wiley & Sons.
2. Modern Electrochemistry by Bockris J.O.M. and Reddy A.K.N., Part I, IIA, IIB, Springer 1998.

3. Electrochemical methods: Fundamentals and applications, by Bard A.J. and Faulkner L.R., John Wiley & Sons, 2002.
4. Electrochemistry, Brett C.M.A. and Brett A.M.O., Oxford University Press, 1993.
5. Principles of electrochemistry, Pilling M.J. and Seakins P.W., Oxford University Press.
6. Chemical Kinetics by K J Laidler, Pearson.
7. Physical chemistry, Atkin P.W., ELBS
8. Kinetics and mechanism of chemical transformation, Rajaraman J and Kuriacose J., Mcmillan
9. Chemical Kinetics & Reaction Dynamics by P L Houston; McGraw Hill International.
10. Chemical Kinetics & Dynamics by J E Steinfeld, J S Franscisco, W L Hase; Prentice Hall International

CHT 105 THERMODYNAMICS 2 CREDITS

UNIT I

1. Laws of thermodynamics: Statistical interpretation of entropy, thermodynamic potentials, chemical potential; thermodynamic properties of ideal gases and mixtures of ideal gases; thermodynamic treatment of non ideal gases. **5L**

2. Reaction equilibrium: Reactions involving gases. Reactions involving pure condensed phases and a gaseous phase; Ellingham diagrams. **5L**

3. Single component phase diagram: Gibbs energies of pure phases and allotropes; Gibbs energy vs. Temperature and pressure; vapour pressure-temperature relation at equilibrium (Clausius - Clapeyron equation). **5L**

UNIT II

4. Binary solutions: Raoultian and Henrian solutions; Thermodynamic properties of ideal solutions; Non-ideal solutions, activity, activity coefficient, Gibbs-Duhem equation, interaction parameters; Regular solution model, concepts of positive and negative deviation, alpha – function. **4L**

5. Partial molar properties & their significance, fugacity: Concepts and determination, properties of ideal solution, non-ideal systems, excess functions for non-ideal solutions, partial molar quantities, determination of partial molar volume and enthalpy. **3L**

6. Statistical thermodynamics: Concept of distribution. Thermodynamic probability. Ensemble averaging, Canonical, grand canonical and micro canonical ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macro states. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. **8L**

Reference Books

1. Physical Chemistry, Atkins P.W., ELBS
2. Physical Chemistry: A molecular Approach, McQuarria D.A. and Simon J.D., University Science Books, Viva books.
3. Thermodynamics & Introduction to Thermostastics by Callen H B
4. Physical Chemistry by Levine Ira N., Tata McGraw Hill, 2007.
5. Physical Chemistry by Atkins P.W and Paula J. De, W.H. Freeman, 2002.
6. Thermodynamics for chemists by Glasstone S.,
7. Principles of Equilibrium Thermodynamics by Denbigh K G
8. McQuarrie, D. A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
9. An introduction to Statistical Thermodynamics by Hill T.L., Dover Publications

CHT 106 COMMUNICATION SKILLS 2 CREDITS

UNIT I

1. Grammar: Conditionals/Tenses, relative clauses, subject–verb agreement, passive voice **6 L**

2. Written communication: Discuss a topic of general interest, but related to science in about 300 words. (Analyze, comment, argue, reflect, persuade, etc.) (can also be used for oral presentations by the students, followed by discussion). **6 L**

3. Oral Communication I: (i) Consulting a dictionary for correct pronunciation (familiarity with phonetics symbols and stress-marks only) (ii) Dialogue **3L**

UNIT II

4. Scientific writing: Writing a Scientific Report on a project undertaken or an experiment conducted (theory + practice) **6 L**

5. Soft Skills

5.1 Gestures/ postures – Body language, gesture, posture. **2L**

5.2 Group discussion – Giving up of PREP, REP Technique, how body language during group discussion. **2L**

5.3 Presentation skills: (i) How to make power point presentation (ii) Body language during presentation (iii) **Resume writing:** Cover letter, career objective, Resume writing (tailor made) **3 L**

5.4 Mock Interview: Each student to face an interview and to demonstrate the above taught skills. **2L**

[**Note:** As regards listening skill it is recommended that a language laboratory be developed and a few sessions be given to the students in the laboratory]

Reference Books:

1. Advanced English Usage; Quirk & Greenbaum; Pearson Education.
2. Developing Communication Skills; Banerjee Meera & Mohan Krishna; Macmillan Publications, 1990.
3. Business Communication; Chaturvedi, P.D.; Pearson Publications.
4. Business Communication; Mathew, M.J.; RBSA Publications, 2005.

5. Communication of Business; Taylor, Shirley; Pearson Publications.
6. Soft Skills : ICFAI Publication
7. Collins English Dictionary and Thesaurus, Harper Collins Publishers and Times Books
8. Longman Language Activator, Longman Group Pvt Ltd
9. Longman Dictionary of contemporary English, Longman
10. The new Penguin Dictionary – a set of dictionaries of abbreviations, spelling, punctuation, plain English, grammer, idioms, thesaurus, 2000.
11. New Oxford Dictionary

CHT 107 MATHEMATICS FOR CHEMISTS 2 CREDITS

UNIT I

1. Basic Trigonometry. **5L**
2. Basic Coordinate Geometry: Cartesian and polar coordinates. **5L**
3. Functions, limits, continuity, Differential and Integral calculus, Differential Equations. **5L**

UNIT II

4. Arithmetic and Geometric progression series, Binomial theorem. **5L**
5. Permutations and Combinations. **5L**
6. Probability and Statistics **5L**

Reference Books

1. Mathematics for Physical Chemistry, R. Mortimer, Academic Press, 2005.
2. Mathematics for physical chemistry, Daniel F., McGraw Hill
3. Chemical Mathematics, Hirst D.M., Longman
4. Mathematics for Chemists, Vol 1, 2, Martin Cockett and Graham Doggett, Royal Society of Chemistry, UK, 2003
5. Chemical calculations – Mathematics for Chemistry, Yates P, CRC Press, 2007.
6. Trigonometry by Loney S.L., Gk Publisher, 2005.
7. Elements of co-ordinate geometry by Loney S.L. Part 1 and 2, All India Traveller Bookseller N Delhi
8. Differential Calculus by Shanti Narayan, S. Chand & Co.
9. Integral Calculus by Shanti Narayan, S. Chand & Co.
10. Higher Algebra by Hall H.S. & Knight S.R.
11. Schaum's Series Books on different topics.

CH 107 BIOLOGY FOR CHEMISTS 2 CREDITS

UNIT I

1. Chemistry of Biological molecules **12L**

1.1 Amino acids: Nomenclature, classification, basic reactions.

1.2 Proteins: Classification, functions, structure characterization.

1.3 Nucleic acids: DNA & RNA: Structures & function.
1.4 Carbohydrates: Structure. Polysaccharides: Structure & function.
1.5 Lipids, Phospholipids, Membrane: Structures & Functions.

2. Cells: Structure of cells, Functions **3L**

UNIT II

3. Light & Life **3L**
4. Bioenergetics: ATP to ADP conversion as a model, Citric acid/ Krebs cycle. **3L**
5. Enzymes, Coenzymes/Cofactors, Kinetics. Use in Organic synthesis, Role of metals. **3L**
5. Secondary Metabolites, Biogenesis. **3L**
6. Applications & Relevance of Biomolecular Sciences in New technologies. **3L**

Reference Books

1. Principles of biochemistry, Lehninger A.L., Nelsen D.L. and Cox M.M., W.H. Freeman, 2004.
2. Chemistry of Biomolecules: An Introduction, Simmonds R.J., Elsevier.
3. Biochemistry, Stryer l, Freeman W.H.
4. Biology for Chemists, Whitemore G., Saujanya Publications, New Delhi, 2006.

CHP 101 INORGANIC CHEMISTRY LABORATORY I 2 CREDITS

(Estimation and Separation Processes)

1. Precipitation – Gravimetry. Precipitation from Homogeneous solution.
2. Paper and Thin Layer Chromatography: For Identification of metal cations and complexes.
3. Solvent Extractions - Metal ion separation. Effect of pH, solvent, time.
4. Ion Exchange – Cation and Anion Exchange.
5. Complexometry – using EDTA and Sequestering agent. Masking and Demasking.
6. Column Chromatography.

CHP 102 ORGANIC CHEMISTRY LABORATORY I 2 CREDITS

(1) Separation of binary mixtures containing monofunctional compounds and identification of the constituents, using microscale techniques.
(2) Purification of compounds by –crystallization, fractional crystallization, distillation, fractional distillation, vacuum distillation, and steam distillation.
(3) Use of TLC for identification of Organic compounds.

CHT 103 PHYSICAL CHEMISTRY LABORATORY I 2 CREDITS

1. Computer in Chemistry - Theory and Usage

(a) Programming Language: Basic knowledge of Fortran 90: Data statements, logical and arithmetic expressions, operators, I-O statements, implementation of loops, control statements, functions & subroutines, array, strings and character processing, format specifications, file processing and data structure.

(b) Numerical Methods: Finding roots of an equation, Newton Raphson method. Basic ideas of interpolation, Newton's forward and backward interpolation. Numerical integration of a definite integral using Trapezoidal and Simpson's one-third rule. Statistical description of data, fast Fourier transform, Fourier and spectral applications. Numerical solution of coupled differential equation using Runge Kutta and Relaxation techniques.

2. Physical Chemistry experiments

(a) Determination of the effect of (i) Change of temperature (ii) Charge of concentration of reactant and catalyst and (iii) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reaction. And determine energy of activation.

(b) Determination of the velocity constant of ionic reaction in micellar media.

(c) Oscillatory reaction.

(d) Verification of Kouhlrasch's Law (Determination of eq. conductivity of a weak electrolyte at infinite dilution)

(e) Verification of Debye -Huckle -Onsager equation.

(f) Determination of activity and activity coefficient of electrolytes.

(g) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.

Reference books

1. Computers in Chemistry, Raman K.V., Tata McGraw Hill
2. Computer programming, Rajaraman V., Prentice Hall.
3. Experiments in Physical chemistry, Shoemaker D.P., Garland C.W. and Nibler J.W., McGraw Hill

SEMESTER II

CHT 201 CHEMISTRY OF TRANSITION METALS 3 CREDITS

UNIT I

1. Metal-Ligand bonding: Valence Bond Theory (VBT), Crystal field theory (CFT) for octahedral, trigonal bipyramidal, square pyramidal, tetrahedral and square planar complexes. Crystal field stabilization energy (CFSE), Factor affecting the crystal field parameters, weak and strong field complexes, spectrochemical series, John-Teller effect. Thermodynamic and related aspects of crystal fields - ionic radii, heats of ligation, lattice energy, site preference energy. Merits and limitations of CFT. Molecular

orbital theory of octahedral, tetrahedral and square planar complexes. Pi bonding in bonding in octahedral complexes. **10L**

2. Metal ligand equilibria in solution: Stepwise and overall formation constants and their interaction, trends in stepwise constants. Factors affecting stability of metal complexes with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin. Determination of binary formation constant by pHmetry and spectrophotometry **5L**

UNIT II

3. Electronic spectra of transition metal complexes: Types of electronic transition, selection rules for d-d transitions. Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes. Calculation of Racah parameters. Charge transfer spectra. Spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information. Inter-valence charge-transfer spectra. **8L**

4. Magnetic properties of transition metals: Different types of magnetic behaviour. Factors affecting observed magnetic moments. Origin of magnetic moment, spin contribution, spin only formulas, orbital contribution, spin-spin coupling. Derivation of van Vleck equation. Methods for magnetic susceptibility measurement, Ferromagnetism and antiferromagnetism, mechanism of anti-ferromagnetic interaction, spin cross over and anomalous magnetic moments. Applications of magnetic measurement for structural elucidation. **7L**

UNIT III

5. Reaction mechanism of transition metal complexes: Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, A, D and I mechanisms for metal complexes, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions. **11L**

6. Compounds with metal-metal multiple bonds and Poly-ions: Metal carboxylate and halide compounds with metal –metal multiple bonds. Isopoly and Heteropoly Acids and salts of V, Mo and W. **4L**

Reference Books:

1.Advanced Inorganic Chemistry, Cotton F.A., Wilkinson G., Murollo C.A. and Bochmann M., John Wiley.
2.Inorganic Chemistry, Huheey J.E., Harper & Row.
3.Chemistry of the Elements. Greenwood N.N. and Earnshaw A., Pergamon.
4.Inorganic Electronic Spectroscopy, Lever A.B.P., Elsevier.
5.Magnetochemistry, Carlin R.I., Springer Verlag.
6.Inorganic Chemistry, Wilysberg G, University Science Books.
7.Physical Methods in Inorganic Chemistry, Drago R. S.

8.Inorganic chemistry, Shriver D. F., Atkins P. W. and Langford C. H., ELBS with Oxford University Press
9.Mechanisms of Inorganic Reactions: Study of metal complexes in solution by Pearson R G, Basolo F., John Wiley & Sons.
10 Inorganic Chemistry : A Unified Approach, by Porterfield William, 2/e, Academic Press an Imprint of Elsevier (Indian Reprint by Rajkamal Electric Press, Delhi.
11. Comprehensive coordination chemistry, eds Wilkinson G, Gillars R.D. and McCleverty J.A., Pergamon.

CHT 202 ORGANIC SYNTHESIS I 3 CREDITS

UNIT I

1. C-C- bond formation: 15L

1.1 Enolate chemistry: Generation: Kinetic and thermodynamic controls in, use of LDA. Aldol reaction, alkylations and acylation reactions of enolates. Michael reaction, Robinson annulation, Mannich reaction, Perkin reaction, Stobbe condensation, Claisen and Dieckmann condensations, Knoevenagel reaction, Reformatsky reaction, Mannich reaction, Grignard reactions, Acyloin condensation, McMurry's coupling reaction.

UNIT II

2. Metal and non-metal mediated oxidation-reductions: 15L

2.1 Mechanism, selectivity, stereochemistry and applications of - Oppenauer oxidations, Aromatization, dehydrogenation, cleavage of C=C bond, ozonolysis, epoxidations using peracids, Baeyer-Villiger oxidation. Oxidations using DDQ, NBS, Pb-tetraacetate, selenium dioxide, Cr & Mn reagents, periodic acid and osmium tetroxide. DMSO-based oxidations. Hydroboration

2.2 Mechanism, selectivity, stereochemistry and applications of Catalytic hydrogenations (using Pd, Pt and Ni catalysts), Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Pondorff-Verley, Dissolving metal reductions, metal hydride reductions ($NaBH_4$, $LiAlH_4$, DIBAL). Wilkinson Rh catalysis, Boron in reduction

UNIT III

3. Designing of synthesis: 10h

1.1 Disconnection approach and Retrosynthetic analysis, ideas of synthons and retrons, Methodology in organic synthesis- Functional group interconversions, general methods of 4 -7 membered ring formation, Examples of acyclic saturated and unsaturated systems, monocyclic and bicyclic compounds.

1.2 Umpolung: concept of umpolung, generation of acyl anion equivalent-1,3-dithiane from carbonyl compounds, use of methylthio-methylsulfoxide, via cyanide ion and cyanohydrin ethers, nitro compounds and metallated vinyl ethers.

1.3 Protection-deprotection of functional groups: Carbonyl, hydroxyl, amino, carboxyl.

4. Enamines: Preparation and synthetic applications. **2L**

5. Ylides: Phosphorus ylides- Wittig reaction and its modifications; phosphine oxides and its applications. Sulphur ylides - preparation and reaction, anions derived from sulfoxides and sulfones. **3L**

Reference books

1. Advanced organic chemistry, Part B, Carey A and Sundberg R.J., Plenum Press.
2. Advanced organic chemistry: Reactions, mechanism and stereochemistry, March J., John Wiley.
3. Theoretical organic chemistry, Parkanyi C., Elsevier
4. Strategic applications of named reactions in organic synthesis, Kurti L. and Czako B., Academic Press, 2005.
5. Organic synthesis, Smith M.B., McGraw Hill, 2002.
6. Organic synthesis: The disconnection approach, Warren S., John Wiley & Sons.
7. Design of organic synthesis, Warren S., Wiley
8. Classics in total synthesis, Nicolaou E.J., Chemie Verlag, 1996
9. The logic of chemical synthesis, Corey E.J. and Cheng X.M., John Wiley & Sons, 1989.
10. Reagents in Organic chemistry, Fieser and Fieser
11. Handbook of reagents in organic synthesis, P Wipf, John Wiley & Sons.
12. Protecting group in Organic synthesis, Greene T, Wuts P.G.M., John Wiley & Sons, 1989.
13. Modern methods of Organic synthesis, Carruther W., Cambridge University Press.
14. Organic synthesis: The science behind art, Smith W.A., Bochkor A.F., Caple, R., RSC, 1998

CHT 203 QUANTUM CHEMISTRY 3 CREDITS

UNIT I

1. Preparatory mathematics 15L

Differential equations and partial differential equation.

Infinite series: Convergence and divergence of infinite series, Taylor series and application, Asymptotic expansion and application, γ, β & error functions, δ functions. Orthogonal polynomials, Legendre, Lagurre and Hermite polynomials & properties.

Matrix algebra: Classification, elementary operations, determinant, rank and inverse of a matrix, solutions of linear equations, eigen functions, eigenvalues, similarity transformations, diagonalization of a matrix.

Vectors: Definitions, dot product, cross product, vector fields, differentiation, line integrals

UNIT II

2. Quantum Chemistry 15L

2.1 Historical background of quantum mechanics, Elementary classical mechanics, linear harmonic oscillator, Classical wave equation, Plane-wave solutions, De Broglie matter waves. Uncertainty principle. Time dependent Schrödinger equation.

2.2 Particle in one dimensional box with infinite and finite walls. Tunneling.

2.3 Operators, Eigenfunctions and Eigenvalues, Operators & quantum mechanics. Degeneracy & average values.

UNIT III

Quantum Chemistry 15 L

2.4 Postulates of quantum mechanics and their analysis.

2.5 Harmonic Oscillator wave function and operator methods.
2.6 Angular momentum: Angular momentum in quantum mechanics in terms of ladder operators. Electron spin; Pauli spin matrices. Spin and magnetic field. Exchange; Slater determinant. Spin-orbit coupling. Spectral term symbols.
2.7 Time dependent and time independent Schrodinger equation and applications to H and He^+ systems, Variational theorem.

Reference Books

1. Mathematics for physical chemists, Mortimer R.G., Elsevier 2005.
2. Mathematical Methods for Physicist by Arfken & Weber, Academic Press, 1995.
3. Mathematical Methods for Scientists and Engineers by McQuarrie, UC DAVIS.
4. Valency, Coulson C.A., ELBS.
5. Physical Chemistry, by Atkins P.W., ELBS.
6. Introduction to Quantum Mechanics with applications to Chemistry by Pauling L. & Wilson E.B., Dover Publications.
7. Introduction to quantum chemistry., Chandra A.K., Tata McGraw Hill
8. Quantum Chemistry by Levine I. N., Prentice Hall, 2000.
9. Molecular Quantum Mechanics by Atkins P.W. and Friedmann R.S., Oxford University Press.
10. Elementary Quantum Chemistry by F. L. Pilar, McGraw-Hill, 1968.
11. Quantum Chemistry by D.A. McQuarrie, Viva books, 2003.
12. Quantum chemistry, Lowe J.P. and Peterson K.Q.C., Academic press, 2005
13. Orbitals in chemistry, Gil V., Cambridge University Press.

CHT 204 ORGANOMETALLIC CHEMISTRY 3 CREDITS

UNIT I

1. Introduction: Types of transition metal to carbon bonds. Classification of organometallic compounds based on hapticity and polarity of M-C bond. Nomenclature and general characters. Synthesis, stability and decomposition pathways. Electron counting and 16 and 18 electron rules - applications and exceptions. **6L**

2. Alkyl and aryl complexes of transition metals: Synthesis, stability and decomposition pathways, organocopper compounds in organic synthesis **2L**

3. Compounds with Metal-carbon multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbines- synthesis, nature of bonds, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis. **7L**

UNIT II

4. Transition metal π-complexes: Transition metal π- complexes with unsaturated organic molecules, CO, alkenes, alkynes, allyl, diene, cyclopentadienyl, arene, cyclooctatrienyl, cyclooctatetraene complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis **13 L**

5. Bimetallic and cluster complexes: Structure and applications in catalysis **2L**

UNIT III

5. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in organometallic compounds – (i) Compounds with acyclic alkenes (ii) Compounds with σ-bonded cyclic alkenes (iii) Compounds with one or more cyclopolyenes π-bonded or σ and π-bonded to several metal atom (iv) Compounds involving rotation of ligands on metals (v) Compounds involving ligands scrambling on metals **8L**

7. Basic organometallic reactions: Ligand substitution, oxidative reactions, migratory reactions, migratory insertion, extrusion, oxidative addition, reductive elimination, reductive elimination –mechanism and stereochemistry. **5L**

8. Importance of organometallic compounds in biological systems **2L**

Reference Books

4. Principles and applications of organotransition metal chemistry, Collman J.P., Hegsdus L.S.,. Nortan J.R. and Finke R.G., University Science Books.
5. The Organometallic chemistry of the transition metals, R.H. Crabtree, John Wiley.
6. Metallo-organic chemistry, Pearson A.J., Wiley.
7. Organometallic chemistry, Mehrotra R.C. and Singh A., New Age International**.**

CHT 205 ORGANIC SYNTHESIS II 3 CREDITS

UNIT I

1. Synthetic methodologies: 15L

1.1 Organosilicons: Important features of silicon governing the reactivity of C-Si compounds: Preparations and important C-C bond forming reactions of alkylsilanes, alkenylsilanes, arylsilanes and allylsilanes. Silylenol ethers as enolate precursors. Silyl as -OH protecting group. Synthetic applications of trialkylsilyl iodide and cyanide.

1.2 Selenium in organic synthesis: preparation of selenols/ selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno-acetals as α-C-H activating groups.

1.3 Selected applications of Samarium iodide and Cerium(IV) in organic synthesis.

1.4 Pd and Rh in organic synthesis: π-bonding of Pd and Rh with olefins applications in C-C bond formations including Wacker process, Heck reaction, Carbonylation, hydroformylation, decarbonylation, olefin isomerism, arylation including aryl amination using Pd reagents. Olefin metathesis using Grubb's catalysts. Sonogashira reaction, Stille coupling, Buchwald reaction and Pauson -Khand reaction.

1.5 Applications of nickel and chromium carbonyls in organic synthesis.

UNIT II

2. Heterocyclic Chemistry 15L

2.1 Nomenclature: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.

2.2 Aromatic heterocycles: Aromaticity, bond lengths, 1H NMR, resonance energy, charge distribution, reactivity, tautomerism.

2.3 Non-aromatic heterocycles: Bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles. Synthesis.

2.4 Small ring heterocycles: Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.
2.5. Five membered heterocycles: Containing two heteroatoms (S,N,O). Diazoles, oxazoles and thiazoles.
2.6 Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzoimidazoles, benzothiazoles.
2.7 Six-membered heterocycles with one heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones.
2.8 Six-membered heterocycles with 2 or more nitrogen atoms: Synthesis and reactions of diazines, triazines.

UNIT III

3 Heterocyclic compounds **5L**

3.1 Seven-membered heterocycles: Synthesis and reactions of azepines, oxepines, thiepines, diazepines, benzodiazepines.
3.2 Heterocycles containing P: Nomenclature, synthesis and characteristics of 5- and 6-membered ring systems: phosphorinanes, phosphorins, phospholanes and phospholes.
3.3 Meso-ionic heterocycles: Classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.

4. Asymmetric synthesis: **10h**

4.1 Principles of asymmetric synthesis.
4.2 Sharpless epoxidation, symmetric dihydroxylation, asymmetric Diels-Alder reactions, Chiral borane reagents, asymmetric reductions of prochiral carbonyl compounds and olefins.
4.3 Use of chiral auxiliaries in diastereoselective reductions. Synthesis of alpha amino acids (Corey's Diastereoselective hydrogenation of cyclic hydrazones); Synthesis of L-DOPA [Knowles's Mosanto process]. Use of Chiral BINOLs, BINAPs and chiral oxazolines and oxazolidones in asymmetric transformations.

Reference books:

1. Transition metals in synthesis of complex organic molecules, Hegedus L, University Science Books, 1999.
2. Heterocyclic Chemistry Vol. 1-3, Gupta R.R., Kumar M.and Gupta V., Springer Verlag.
3. The Chemistry of Heterocycles, Eicher T.and Hauptmann S., Thieme.
4. Heterocyclic chemistry Joule J.A., Mills K, Blackwell Publishing, 2008.
5. Heterocyclic Chemistry, Gilchrist T.L., Longman Scientific Technical.
6. Contemporary Heterocyclic Chemistry, G,.R. Newkome and W.W. Paudler, Wiley-Inter Science.
7. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiely.
8. Comprehensive Heterocyclic Chemistry, Katrizky A.R. and Rees C.W., eds. Pergamon Press.
9. Stereoselective synthesis, Atkinson R.S., John Wiley & Sons, 1995
10. Principles of Asymmetric synthesis, Gawley R.E., Aub J., Elsevier.

11. The chemistry of phosphorus, Emsley and Hall
12. Name reactions in heterocyclic chemistry, LI J.J., Wiley Interscience, 2005.
13. Asymmetric Synthesis - The Essentials, Mathias Christmann, Stefan Bräse, Wiley-VCH

CHT 206 GROUP THEORY & SPECTROSCOPY 3 CREDITS

UNIT I

1. Group theory 15L

1.1 Groups, subgroups & classes.
1.2 Symmetry elements, operations & associated algebra.
1.3 Elements of group theory: Dipole moment & optical isomerism.
1.4 Symmetry point groups, symmetry classification of molecules with examples.
1.5 Representation of point groups, reducible & irreducible representations, Great orthogonality theorem, construction of character table, reduction formula, direct product, projection operator, symmetry adapted linear combinations.

UNIT II

2. Spectroscopy 15L

2.1 Rotational & vibrational spectroscopy: Intensity & width of a spectral line.
2.2 Electromagnetic spectrum, Einstein's coefficient of spontaneous emission, transition moments & selection rules.
2.3 Types of rotors, pure rotational spectra & energy levels, Stark effect, Rotational Raman spectra.
2.4 Selection rules for vibrational spectrum, anharmonicity, vibration-rotation spectra & spectral branches. Normal modes and vibrations of polyatomic molecules, exclusion principle.

UNIT III

Spectroscopy 15L

2.5 Electronic spectroscopy: Nature of transition, Franck-Condon factor, Quantum yield and radiative processes, Fluorescence & Phosphorescence.
2.6 Elementary ideas of laser and laser action, Applications in chemistry.
2.7 Symmetry aspects of molecular orbital theory with examples. Hybrid orbitals & molecular orbitals. Symmetry of normal modes, normal mode analysis, selection rule for IR & Raman transitions.

Reference Books

1. Group theory in chemistry by Bishop, Dover.
2. Chemical applications of group theory by Cotton, John Wiley.
3. Introduction to molecular spectroscopy by G Barrow
4. Symmetry in molecules by Hollas J.M., Chapman.
5. Symmetry in chemistry, Jaffe H.H. and Orchin M., Dover Publications, 2002
6. Chemical applications of group theory, Cotton F.A., Wiley International, 1990

7. Symmetry and spectroscopy: An introduction to vibrational and electronic spectroscopy, Harris D.C. and Bertolucchi M.D., Dover Publications, 1990
8. Molecular Spectroscopy by P W Atkins
9. Molecular spectroscopy, Machale J., Prentice Hall, 1999
10. Molecular spectroscopy, Hollas, J.M., John Wiley
11. Fundamentals of molecular spectroscopy by C. W. Banwell and McCash, E., Tata McGraw Hill, 1999
12. Physical methods for chemists by R S Drago

CHP 202 INORGANIC CHEMISTRY LABORATORY II 2 CREDITS

Synthesis, characterization and estimation of metal ions using any of UV-VIS/IR and magnetic measurements in the following:
(i) $VO(acac)_2$ (ii) *cis and trans* -$K[Cr(C_2O_4)_2(H_2O)_2]$ (iii) $Na[Cr(NH_3)_2(SCN)_4]$
(iv) $Mn(acac)_3$ Fe(acac)3 (Green Method) (v) $K_3[Fe(C_2O_4)_3]$ (vi) $[Co(NH_3)_6]$ $[Co(NO_2)_6]$
(vii) *cis*-$[Co(trien)\ (NO_2)_2]$ $Cl.H_2O$ (viii) $Hg[Co(SCN)_4]$ (ix) $[Ni(NH_3)_6]Cl_2$
(x) $[Cu(NH_3)_4]SO_4.H_2O$

Reference books

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge University Press, 1970.
2. Synthesis and Characterisation of Inorganic Compounds, W. L. Jolly, Prentice Hall.
3. Inorganic Preparations: a systematic course of preparations by Alexander King, London, T. Murphy

CHP 202 ORGANIC CHEMISTRY LABORATORY II 2 CREDITS

1. Single and two step organic synthesis involving important named reactions, new reagents, new methodology, green principles, stereochemistry. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, E-factor, etc. should be paid attention to. TLC should be used to monitor the reaction and finding out the purity of the product.
2. Estimation of organic compounds

Reference books:

1. Organic chemistry experiments: Microscales and semimicroscales, Campbell, B.N. and Ali M, McCarty M, Brooks/Cole, 1994.
2. Techniques and experiments for organic chemistry, Ault A., University Science Books, 1998.
3. Multiscale operational organic chemistry: A problem solving approach to laboratory course, Lehman, Prentice Hall, 2002.

4. Green chemistry experiments, Green Chemistry Network Centre, University of Delhi, Delhi.
5. Monograph on green chemistry laboratory experiments, Green chemistry task force committee, DST, New Delhi.

CHP 203 PHYSICAL CHEMISTRY LABORATORY II 2 CREDITS

1. Determination of the dissociation constant. Determination of molecular weight of non-volatile and electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
2. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
3. Acid-base titration in a non-aqueous media using a pH meter.
4. **Polarimeter:** Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter. Enzyme kinetics-inversion of sucrose.
5. **Chromatography:** Thin-layer chromatography-separation of nickel, manganese, cobalt and zinc. Determination of Rf values.

SEMESTER III

CHT 301 SPECTROSCOPY 3 CREDITS

UNIT I

1. UV-VIS spectroscopy - Woodward-Fieser rules, UV spectra of aromatic and heterocyclic compounds **3L**

2. IR and Raman spectroscopy: FT technique, group frequencies, vibrational coupling. NIR spectroscopy. Scattering phenomena. Raman spectroscopy. **5L**

3. Mass spectrometry: Basics. Ion production: EI, CI, FD, FAB. Ion analysis techniques. Isotopic abundance, ion abundance. Molecular ion peak, metastable peak, nitrogen rule. Common fragmentation modes, rearrangement of ions. HRMS. **7L**

UNIT II

4. NMR spectroscopy: Basic theory. Pulse technique and FT. **H1 NMR:** Chemical shifts and factors affecting the same, spin-spin coupling of different systems. Simplification of complex spectra- Deuterium exchange, double resonance, shift reagents, NOE. **C13 NMR:** Basics, chemicals shifts. **2D NMR –** COSY, NOESY, DEPT, INEPT, APT and INADEQUATE.. **F19 and P31 NMR.** Solid state NMR. **15L**

UNIT III

5. ESR spectroscopy: Theory, experimental technique, Hyperfine splitting, ESR parameters, **2L**

6. Hyphenated techniques: GC-MS, LC-MS, HP-TLC**.** **5L**

7. Mossbaur spectroscopy: Basics, spectral parameters and spectral display. Applications. **3L**

8. Emission: Flame photometry, ICP, Ark-Spark spectra, Phosphorescence, XRF **3L**
9. ORD and CD: Introduction, determination of absolute configuration **2L**

Structure elucidation using combined stereoscopic methods

Books Recommended

1. Practical NMR Spectroscopy, Martin M.L., Deepish J.J. and Martin G.J., Heyden.
2. Spectrometric Identification of Organic Compounds, Silverstein R.M., Bassler G.C. and Morrill T.C., John Wiley.
3. Introduction to NMR spectroscopy, Abraham R.J., Fisher J. and Loftus P., Wiley.
4. Application of Spectroscopy of Organic Compounds, Dyer J.R. Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry Williams D.H., Fleming I., Tata McGraw-Hill.
6. Organic Spectroscopy, Kemp W., W.H. Freeman & Co.
7. Spectroscopy, Pavia D. L., Lapman G.M., Kritz G.S., and Vyvyan J.R., Brooks/Cole (Indian Reprint), 2009.
8. Modern NMR techniques for Chemistry Research, Derome A. E., Pergamon.

PHOTOCHEMISTRY, PERICYCLIC REACTIONS AND CARBOCYCLIC RING SYSTEMS

CHT 302 **3 CREDITS**

UNIT I

1. Photochemistry: **15h**

1.1 Photochemical reactions: Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

1.2 Determination of reaction mechanism: Classification, rate constants and life times of reactive intermediates. Determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions-photo dissociation, gas-phase photolysis.

1.3 Photochemistry of alkenes: Intramolecular reactions of the olefinic bond –cis-trans isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

1.4 Photochemistry of carbonyl compounds: Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, β,γ-unsaturated and α, β-unsaturated compounds, cyclohexadienones. Intermolecular cyloaddition reactions-dimerisations and oxetane formation.

1.5 Photochemistry of aromatic compounds: Isomerisations, additions and substitutions.

1.6 Miscellaneous photochemical reactions: Photo-Fries reaction of anilides, Photo-Fries rearrangement. Barton reaction. Singlet molecular Oxygen reaction. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

UNIT II

2. Pericyclic reactions **15L**

2.1 Molecular orbitals: MOs of acyclic and cyclic polyenes and arenes. FMO. Role of FMO in organic reactions.

2.2 Pericylic reactions: Classification of pericyclic reactions. Thermal and photochemical reactions. **Three approaches:** Conservation of orbital symmetry and correlation diagram, Frontier molecular orbital approach [FMO] and Aromatic (Huckel and Mobius) transition state approach.

2.3 Cycloaddition reactions: 4n and 4n+2 π electron systems. Diels-Alder reactions, 1,3-Dipolar cycloadditions and cheletropic reactions, the ene reactions.

2.4 Electrocyclic reactions: Conrotatory and disrotatory motions, 4n and 4n+2 π electron systems and other systems. Valence tautomerism.

2.5 Sigmatropic rearrangements: H-shifts and alkyl-shifts, supra and antarafacial migrations. Cope and Claisen rearrangements. Degenerate Cope rearrangement, Fluxional tautomerism. Wittig rearrangement, 2,3-sigmatropic shifts.

UNIT III

3. Carbocyclic ring systems. **15L**

1. Nomenclature of polycyclic ring systems
2. Baldwin rules for ring closure. Bredt rule
3. Synthesis of small and large ring systems: Ring strains, entropy consideration in ring closure.
4. Dieckmann condensation, Bergman cyclization, Nazarov cyclization, palladium mediated cyclizations, radical cyclizations, Simmons-Smith procedure in formation of cyclopropane ring and ring expansion, Favorskii reaction, Curtius reaction, Scmidt reaction, oligomerization of alkynes and conjugated dienes, Ring contraction and expansion, ring metathesis.

Reference books

6. Essentials of Molecular Photochemistry, Gilbert A and Baggott J., Blackwell Scientific Publication.
7. Molecular Photochemistry, Turro N.J., W.A.Benjamin.
8. Introductory Photochemistry, Cox A.and Camp T., McGraw Hill.
9. Molecular orbitals and photochemical reactions, Fleming I.
10. Advanced organic chemistry, Carey and Sundberg, Plenum.
11. Photochemistry, Kundall R.P. and Gilbert A., Thomson Nelson.
12. Organic Photochemistry, Coxon J. and Halton B., Cambridge University Press.
13. Orbital interaction in chemistry, Albright T., Burdee J and Whango M, Wiley VCH
14. Pericyclic reactions, Mukherji S.M., Mcmillan

CHP 303 BIOMOLECULAR CHEMISTRY 3 CREDITS

UNIT I

1. Nature of biomolecular Interactions -Non-covalent, hydrophobic, binding constants & its implications. **4L**

2. Chemical and enzymatic methods of synthesis of proteins. **6L**

3. Molecular mechanisms of enzymatic process. Concept of enzyme inhibitor as

drugs. **5L**

UNIT II

4. DNA organization, replications, transcription-translation. **3L**
5. Chemical and enzymatic methods of DNA/RNA synthesis. **5L**
6. Interactions of small molecules with DNA/proteins. **4L**
7. Lipids, Biomembrane; Organization, membrane bound proteins, Transport phenomenon. **3L**

UNIT III

8. Post Translation Modifications & their Significance. **2L**
9. Molecular biology - Recombinant DNA, PCR and their Applications, Smart biomaterials. **5L**
10. Role of metals in biology. **3L**
11. Analysis of biomolecules (Chiroptic, emission, mass etc.) **5L**

Reference books

1. Biochemistry: The chemical reactions of living cells, Metzler D.E., Academic Press.
2. DNA structure and function, Sinden R.P., Academic Press

CHT 304 ENVIRONMENTAL CHEMISTRY 3 CREDITS

UNIT I

1. General aspects of environment: Environmental components (atmosphere, hydrosphere, lithosphere and biosphere); Composition of air, water, soil; Atmosphere and its interaction with hydrosphere, lithosphere and biosphere. Vertical temperature and vertical structure of the atmosphere. **4L**

2. Environmental pollution- Types & classification of pollutants. Biogeochemical cycles in environment – Detail study of nitrogen cycle; Biological Control of chemical factors in the environment; Generation and decomposition of pollutants in nature. Biodistribution of elements. Chemical and photochemical reactions in atmosphere; Effects and control of air pollutants-Gaseous, particulates. Environmental impact assessment, environmental modeling and environmental laws **8L**

3. Green house effect : Green house gases - Major sources and effect, effect on global warming and agriculture. **3L**

UNIT II

3.2 Earth's carbon cycle, carbon emitters, carbon sequestration, carbon footprint and carbon trading. **3L**

3.3 Ozone depletion: Ozone layer – Formation, reactions, role, and processes of ozone depletion. Consequences of ozone depletion. **3L**

4. Environmental toxicology: Introduction; threshold limiting value (TLV); Toxicity and control of toxicants-- Nonmetallic compounds, asbestos, organic compounds,

endocrine disrupters, persistent organic pollutants (POP's), polychlorinated biphenyls (PCB's), dioxins, pesticides, phthalates, heavy metals- As, Hg, Cd, Pb. **4L**

5. Renewable energy: Alternative clean fuels- Solar, biomass energy, hydrogen, hydrothermal, geothermal, wind, etc. **3L**

6. Climate change in future: Predictions, consequences. Mitigation and adaptation to climate change. Montreal protocol 1987, Rio de Janeiro summit 92 Kyoto protocol 97, Johannesburg 2002, Copenhagen summit 2009. **2L**

Reference Books:

1. Environmental Chemistry, Manahan S. E., CRC Press, 2010
2. Environmental Chemistry, Colin Baird, Michael Cann; Fourth Edition;W.H. Freeman and Company, New York, 2008.
3. Environmental Chemistry, De A.K.; Fourth Edition; New Age International Pvt. Ltd., New Delhi, 2003.
4. Chemistry of the Environment, Spiro T. G. & William M. Stigliani; Second Edition; Prentice-Hall of India Pvt. Ltd., New Delhi, 2002.
5. Environmental Chemistry, Gary W. V. & Stemphen D. J.; A Global Perspective; Oxford University Press, New York, 2000.
6. Global Warming Green House Gases Worldwide impacts, Julie Kerr casper.
7. Fundamentals of sustainable science, Manahan E., CRC Press., 2009.
8. Environmental chemometrics – Principles and modern applications, Hanrahan G, 2009.
9. Basic concepts of environmental chemistry, Connell D.W., CRC Press, 2006

CHT 305 GREEN CHEMISTRY I 3 CREDITS

UNIT I

1. **Green chemistry:** History, need, and goals. Green chemistry and Sustainability. Dimensions of sustainability, Limitations/Obstacles in pursuit of the goals of Green Chemistry. Opportunities for the next generation of materials designers to create a safer future. **5L**

2. Basic principles of Green Chemistry and their illustrations with examples. **10L**
   (i) Prevention of waste/byproducts.
   (ii) Maximum Incorporation of the materials used in the process into the final product (Atom Economy): Green metrics
   (iii) Prevention/Minimization of hazardous/toxic products.
   (iv) Designing safer chemicals - different basic approaches
   (v) Selection of appropriate auxiliary substances (solvents, separation agents etc)
   (vi) Energy requirements for reactions—use of microwave, ultrasonic energy
   (vii) Selection of starting materials—use of renewable starting materials.
   (viii) Avoidance of unnecessary derivatization—careful use of blocking/protection groups.

(ix) Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents.
(x) Designing biodegradable products.
(xi) Prevention of chemical accidents.
(xii) Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

UNIT II

3. Examples of green synthesis/reaction: 15L

3.1 Green starting materials
3.2 Green reagents
3.3 Green solvents and reaction conditions
3.4 Green catalysis
3.5 Green synthesis- Real world cases

(Traditional processes and green ones)
Synthesis of Ibuprofen, Adipic acid etc and selected examples from US Presidential Green Chemistry Challenge Award Winners.

UNIT III

4. Hazard assessment and mitigation in chemical industry

5. Future trends in Green Chemistry: Oxidation-reduction reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Noncovalent derivatization. Biomass conversion, emission control. Biocatalysis **15L**

Reference Books:

1. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press.
2. Green Chemistry: Introductory Text. M. Lancaster Royal Society of Chemistry (London).
3. Introduction to Green Chemistry. M.A. Ryan and M.Tinnesand, American Chemical Society (Washington).
4. Real world cases in Green Chemistry, M.C. Cann and M.E. Connelly. American Chemical Society (Washington).
5. Real world cases in Green Chemistry (Vol 2) M.C. Cann and T.P.Umile. American Chemical Society (Washington)

CHT 308 PROJECT PREPARATION

Candidate will be given a topic of project at the beginning of Semester III. The candidate is expected to collect pertinent literature and make a presentation based on the literature and the proposed plan of work at the end of Semester III.

PRACTICALS

CHP 301 INORGANIC CHEMISTRY LABORATORY III 2 CREDITS

Instrumental methods

(i) Spectrophotometric determination of manganese/chromium/vanadium in steel sample.
(ii) Nickel/molybdenum/tungsten/vanadium/uranium by extractive spectrophotometric method.
(iii) Fluoride/nitrite/phosphate.
(iv) Determination of stoichiometry of zirconium-alizarin Red-S complex : Mole-ratio method.
(v) Determination of stoichiometry of copper-ethylenediamine complex : Slope-ratio method.
(vi) Determination of stoichiometry of iron-phenanthroline complex : Job's method of continuous variations.
(vii) Flame photometric determinations of - sodium and potassium when present together; lithium/calcium/barium/strontium; calcium and magnesium in tap water.
(viii) Determination of stability constant of a complex by pH metry
(ix) Determination of metal ions in a mixture sample by AAS.

Reference books

1. Vogel's Textbook of Quantitative Analysis, revised J. Bassett, R. C. Denney, G.H. Jeffery and J.Mendham, ELBS.
2. Laboratory manual: Analytical Chemistry - principles and techniques by Larry G. Hargis, Prentice Hall.

CHP 302 ORGANIC CHEMISTRY LABORATORY III 2 CREDITS

(1) Extraction of natural products. Use of column chromatography for separation and purification.
(2) Synthesis of compounds through three or more steps.
(3) Estimations of Organic compounds
(4) Use of instrumental methods for identification/characterization of compounds

Reference Books:

1. Organic chemistry experiments: Microscales and semimicroscales, Campbell, B.N. and Ali M, McCarty M, Brooks/Cole, 1994.
2. Techniques and experiments for organic chemistry, Ault A., University Science Books, 1998.
3. Multiscale operational organic chemistry: A problem solving approach to laboratory course, Lehman, Prentice Hall, 2002.

CHP 302 PHYSICAL CHEMISTRY LABORATORY III 2 CREDITS

(i) Determination of thermodynamic constants, ΔG, ΔS, and ΔH for the reaction by e.m.f. method. $Zn + H_2SO_4 \rightarrow ZnSO_4 + 2H$
(ii) Determine and compare surface tension values of detergents of different trade mark.

Spectroscopy

(iii) Determination of composition of KMnO4+K2Cr2O7 solution
(iv) Determination of pKa of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media
(v) Manganese/Chromium/Vanadium in steel sample.
(vi) Nickel/ molybdenum/ tungston/ vanadium/ uranium by extractive spectrophotometric method.
(vii) Fluoride/nitrite/phosphate.

Flame Photometry

(viii) Sodium and potassium when present together.
(ix) Lithium/calsium/barium/strontium.
(x) Cadmium and magnesium in tap water.

Chromatography

(xi) Thin-layer chromatography-separation of nickel, manganeses, cobalt and zinc. Determination of Rf values.

SEMESTER IV

CH 401 GREEN CHEMISTRY-II 3 CREDITS

UNIT I

1. **Green solvents** **10 L**

1.1 Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability.
1.2 Ionic liquids
1.3 Supercritical fluids
1.4 Solvent free neat reactions in liquid phase

1.5 Solvent free solid phase reactions
1.6 Flourous phase reactions

2. Nonconventional energy sources 5L

2.1 Microwave assisted reaction
2.2 Ultrasound assisted reactions
2.3 Photochemical reactions using sunlight

UNIT II

3. Green catalysis 15L

3.1 Heterogeneous catalysis: Use of zeolites, silica, alumina, clay, polymers, cyclodextrin, and supported catalysts.
3.2 Biocatalysis: enzymes, microbes etc
3.3 Phase-transfer catalysis (micellar/ surfactant etc)

UNIT III

4. Green industrial processes- case studies **5L**
5. Green analytical methods **5L**
Tutorials/Assignment/Visiting Lectures: **5L**

(Throughout the semester there will be some visiting lecturers that will talk about an area related to the topic.)

Reference books:

15. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press.
16. Green Chemistry: Introductory Text. M. Lancaster Royal Society of Chemistry (London).
17. Introduction to Green Chemistry. M.A. Ryan and M.Tinnesand, American Chemical Society (Washington).
18. Real World Cases in Green Chemistry . M.C. Cann and M.E. Connelly. American Chemical Society (Washington).
19. Real World Cases in Green Chemistry(Vol 2) . M.C. Cann and T.P.Umile. American Chemical Society (Washington).
20. Alternative Solvents for Green Chemistry. F.M. Kerton. Royal Society of Chemistry (London).
21. Recoverable and Recyclable Catalysts. M. Benaglia. Wiley.
22. Handbook of Green Chemistry & Technology. J. Clark and D. Macquarrie. Blackwell Publishing.
23. Solid-Phase Organic Synthesis. K. Burgess. Wiley-Interscience.
24. Eco-Friendly Synthesis of Fine Chemicals. R.Ballini. Royal Society of Chemistry (London)

SOLID STATE, SURFACES, & CATALYSIS

CHT 402 **3 CREDITS**

UNIT I

1. Solid state chemistry **15L**

Crystal structure, crystal types, crystal defects. Electronic structure of solids – Band theory. Superconductivity. Theory of insulators, semiconductors and metals. Optical and magnetic properties. Alloys. Solid state reactions

UNIT II

2. Surface Chemistry **15L**

Surface excess properties and thermodynamics. Surface tension, capillary action, Adsorption: Thermodynamics and kinetics. Estimation of surface area (BET). Surface films on liquids. Catalytic activity at surface. Surface active agents and various aggregations of them in aqueous solutions, CMC and factors affecting CMC. Thermodynamics of micellization. Microemulsions.

Surface characterization: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XANES, XRD TPD etc.

UNIT III

3. Catalysis **15L**

1. Types of catalysis: Heterogeneous and Homogeneous catalysis, advantages and disadvantages. Catalytic cycles.

2. Heterogeneous catalysis: Preparation methods, characterization and quantification of surface active sites, kinetics of heterogeneous catalytic reactions. Structure of adsorbed species. Supported catalysts and metal-support interaction. Catalyst deactivation and regeneration

3. Homogeneous catalysis: Homogeneous acid-base catalysis. Hydrogenation, hydroformylation, hydrocyanation, hydrosilylation, Wilkinson catalysts, Chiral ligands and chiral induction, Ziegler-Natta catalysts

4. Organometallics as catalysts: Bonding and structure transition metal complexes, applications in reactions such as hydrogenation, carbonylation, coupling reactions - Suzuki coupling, Heck coupling and related cross coupling reactions. Alkene oligomerization and metathesis. Catalytic oxidations and reductions, epoxidation, dihydroxylations, decarbonylation, olefin isomerization, arylation, polymerization, asymmetric synthesis, heterogenised homogeneous catalysts.

Reference books

4. Solid state chemistry and its applications, West A.R., Plenum.
5. Principles of solid state, Keer H.V., Wiley Eastern
6. Solid state chemistry, Chakrabarty D.K., New Wiley Eastern
7. Solid state chemistry: An introduction, Moore E., and Smart L., Chapman Hall, 1996
8. Crystallography made crystal clear: A guide for users of macromolecular models, Rhodes G., Elsevier, 2006.
9. X-ray diffraction, Warren B., Dover Publications
10. Introduction to crystallography, Sands, D.E., Dover Publications.
11. Homogeneous transition metal catalysis, Masters C., Chapman & hall.
12. Principles and practice of heterogenous catalysis, Thomas J.M. and Thomas M.J., John Wiley
13. Concepts of modern catalysis and kinetics, Chorkendoff I.B. and Niemantsverdriet J.M.

14. Physical chemistry of surfaces, Adamson A.W., Wiley Interscience, 1997

CHP 401 PROJECT

A student is assigned 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 as the prescribed norms.

9. ELECTIVES UNDER CORE COURSES

Courses from the following list may be offered depending upon the expertise available within the School.

1) Statistical Thermodynamics
2) Advanced Quantum Chemistry
3) Interfacial Chemistry
4) Computational Chemistry
5) Bioinorganic Chemistry
6) Bioorganic Chemistry
7) Physical Organic Chemistry
8) Natural Products
9) Polymer Chemistry
10) Nuclear Chemistry
11) Medicinal Chemistry
12) Chemical Reaction Engineering
13) Material Chemistry
14) Advanced Electrochemistry
15) Industrial Organic Chemistry
16) Supramolecular Chemistry
17) Irreversible thermodynamics

10. ELECTIVES UNDER SUPPORTIVE/SOCIALLY ORIENTED COURSES

Courses from the following list may be offered depending upon the expertise available within the University.

1) Basic electronics & Instrumentation
2) Financial management
3) Industrial management
4) Rural development

5) Ethics in Science & Technology
6) IPR
7) Philosophy of Science
8) History of Chemistry
9) Archiometallurgy
10) Safety, Hygene and Environment
11) HRD
12) Indology