SIDHO-KANHO-BIRSHA UNIVERSITY

Syllabus for M. Sc. Course in Chemistry

Effective from the session 2011-12

Distribution of papers and marks

(A) SEMESTER-I

THEORETICAL (General paper)	Division of Marks Subtotal: 200	Lecture Hours.	Exam. Hrs.
CH 101 (General Chemistry)	50	60-65	3
CH 102 (Inorganic Chemistry)	50	60-65	3
CH 103 (Organic Chemistry)	50	60-65	3
CH 104 (Physical Chemistry)	50	60-65	3

PRACTICAL	Division of Marks Subtotal:100	Lab. Hours Subtotal: 200	Exam. Hrs.
CH 105 (Inorganic general)	30+20 = 50	100	6
CH 106 (Organic general)	30+20 = 50	100	6

(30 marks for experiments, 20 marks for continuous assessment (Quiz, attendance, performance, etc.)

(B) SEMESTER-II

THEORETICAL (General paper)	Division of Marks Subtotal: 200)	Lecture Hours.	Exam. Hrs.
CH 201 (Analytical Chemistry)	50	60-65	3
CH 202 (Inorganic Chemistry)	50	60-65	3
CH 203 (Organic Chemistry)	50	60-65	3
CH 204 (Physical Chemistry)	50	60-65	3

PRACTICAL	Division of Marks Subtotal:100	Lab. Hours Subtotal: 200	Exam. Hrs.
CH 205 (Physical general)	30+20 = 50	100	6
CH 206(Analytical & data Processing)	30+20 = 50	100	6

(30 marks for experiments, 20 marks for continuous assessment (Quiz, attendance, performance, etc.)

(C) SEMESTER-III

THEORETICAL	Division of Marks Subtotal:200	Lecture Hours.	Exam.Hrs.
CH 301 (Advanced General I)	50	60-65	3
CH 302 (Advanced General II)	50	60-65	3
CH 303 (Advanced General III)	50	60-65	3
CHI/CHO/CHP 304(Special Paper)	50	60-65	3

PRACTICAL	Division of Marks Subtotal: 100	Lab. Hours Subtotal: 200	Exam. Hrs.
CHI/CHO/CHP 305 (Special Paper)	30+20 = 50	100	6
CHI/CHO/CHP 306 (Special Paper)	30+20 = 50	100	6

(30 marks for experiments, 20 marks for continuous assessment (Quiz, attendance, performance, etc.)

(D) SEMESTER-IV

THEORETICAL	Division of Marks (Subtotal:200)	Lecture Hours.	Exam. Hrs.
CHI/CHO/CHP 401 (Special Paper)	50	60-65	3
CHI/CHO/CHP 402 (Special Paper)	50	60-65	3
CHI/CHO/CHP 403 (Special Paper)	50	60-65	3
CHI/CHO/CHP 404 (Special Paper)	50	60-65	3

PRACTICAL	Division of Marks Subtotal: 100 `	Lab. Hours Subtotal: 200	Exam. Hrs.
CHI/CHO/CHP 405 (Special Paper)	30+20 = 50	100	6
CHI/CHO/CHP 406 (Special Paper)	30+20 = 50	100	6

30 marks for experiments/project work, 20 marks for continuous assessment (Quiz, attendance, performance, etc.)/seminar lecture.

Semester-I

Theoretical

CH 101: General Chemistry

Group A

1. Nuclear properties and structure: (22 lectures)
Introduction to nuclear stability, formulation of semi-empirical binding energy equation, mass parabola and application of binding energy equation; nuclear reactions, Q value and cross section of nuclear reaction, compound nucleus theory (qualitative approach), calculation of fission probability using binding energy equation, shell model, nuclear magic number and its derivation from nuclear potential well, calculation of nuclear spin, nuclear isomerism and non-optical transitions; Synthetic elements; theoretical background, production of super heavy elements.

2. Radioactive equilibrium: (10 lectures)
Successive disintegration, Bateman equation, secular and transient equilibrium, no equilibrium; analysis of special types of successive disintegration, formation of radioelement in a nuclear reaction, activation analysis.

Group B

3. Environmental chemistry: (17 lectures)
Characteristics of atmosphere, radiation balance; Greenhouse effect monitoring, mechanistic pathways of smog formation and ozone hole, acid rain; major, minor and trace constituents of the atmosphere; water quality parameters, biochemical effects of As, Pb, Cd, Hg, organic toxicants, pesticides and their chemical speciation; eutrophication, waste water treatment—primary, secondary and tertiary treatment, nuclear waste; nuclear accidents, control of air pollution: different methods — gravitational setting chamber, cyclone separators, electrostatic precipitation; role of plants, various sources of soil pollution; noise pollution: classification, hazards.

4. Application of Statistics to Data Treatment and Evaluation: (13 lectures)
Significance Test – Paired, one tailed and two tailed t-test, F-test, Q-test for outliers, ANOVA and chi-squared test, Estimation of detection limits, Least square method for calibration plots, Quality assurance and controlled charts, Regression and correlation analysis.

Recommended Books/Journals

H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edn Reprint, New Age International (P) Ltd Publications,New Delhi, 2001.
R. D. Evans, *The Atomic Nucleus*, McGraw-Hill, New York, 1979.
B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice Hall, 1965.
S. Glasstone, *Source Book of Atomic Energy*, East-West Press Private Ltd, New Delhi, 1967.
G. R. Choppin and J. Rydberg, *Nuclear Chemistry: Theory and Applications,* Pergamon Press, Oxford, 1980.
G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*, 3rd Ed., Jhon Wiley & Sons Inc., New York, 1981.
D. D. Sood, A.V. R Reddy, N. Ramamoorty, *Fundumentals of Radiochemistry*, Yancas, Mumbai, 2004
V. I. Goldanskii and R. H. Herber, *Chemical Applications of Mossbauer Spectroscopoy*, Academic Press, New York, 1968.
N. N. Greenwood and T. C. Gibb, *Mossbauer Spectroscopy*, Chapman and Hall, London, 1971.
C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.
R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.
R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

CH 102: Inorganic Chemistry

Group A

1. Valency theories: quantum chemical approach: (15 lectures)
Variation method, LCAO and Huckel approximation applied to H_2^+ and H_2 type systems, sigma and pi MO's (ethylene, allyl systems, butadiene, benzene etc.); comparative study of the application of VB and MO methods to diatomic species; MO of polyatomic molecules; Walsh diagram, configuration interaction, orbital construction for Hn type systems, isolobal analogy.

2. Coordination chemistry: bonding, stereochemistry and structure: (16 lectures)
Introduction to Crystal Field Theory, ligand field theory, molecular orbital theory; 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, complex equilibria, Labile and inert complexes, Introduction to stability constant.

Group B

3. Cluster compounds: (14 lectures)
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.

4. Bioinorganic chemistry: (17 lectures)
Metal ions in biology, myoglobin, heamoglobin, heamocyanin, hemerythrin, cytochromes, rubredoxin, feredoxins; biological fixation of nitrogen, chlorophyll and photosynthesis; PS-I, PSII, bioenergetics and ATP cycle, glucose storage, Na+/K+ ion pump, ionophores, DNA polymerization, metal ion interaction with nucleoside and nucleotide; metal-protein interaction- storage, transfer and activity; study of metalloprotein and metalloenzyme catalase, peroxidase, ceruloplasmin, cytochrome oxidase, carbonic anhydrase, carboxy peptidase, metallothionine, xanthine oxidase, sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; vitamin B12 and B12-enzyme; toxicity and detoxification of metal ions; chelation therapy.

Recommended Books/Journals

R. McWeeney, *Coulsons' Valence*, 3rd. Edn, Oxford University Press, Oxford, 1979.
T. A. Albright, J. K. Burdett and M. H. Whangbo, *Orbital Interactions in Chemistry*, Wiley, New York, 1985.
K. Fukui and Fujimoto, *Frontier Orbital and Reaction Paths,* World Scientific, Singapore, 1995
G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
D. F. Shriver, P. W. Atkins and C. H. Langford, *Inorganic Chemistry*, Oxford University Press, New York,1990.
B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley and Sons, Inc., New York, 2001.
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.
T. P. Fehlner, J. –F. Halet and J. –Y. Saillard, *Molecular Clusters — A Bridge to Solid State Chemistry*, Cambridge University Press, Cambridge, 2007.
M. Driess and H. Noth (Eds.), *Molecular Clusters of the Main Group Elements,* Wiley-VCH, Weinheim, 2004.
D.M.P. Mingos and D.J.Wales, *Introduction to Cluster Chemistry*, Prentice Hall, New York, 1990.
D.M.P. Mingos (Ed.), *Structural and Electronic Paradigms in Cluster Chemistry*, Springer, Berlin, 1997.
D.F. Shriver, H.D. Kaesz and R.D. Adams (Eds.), *The Chemistry of Metal Cluster Complexes*, VCH, New York, 1990.
P. Braunstein, L. A. Oro and P. R. Raithby (Eds.), *Metal Clusters in Chemistry*, Wiley-VCH, Weinheim, 1999.
M. H. Chisholm (Ed.), *Early Transition Metal Clusters with π-Donor Ligands*, VCH, New York, 1995.
K.J. Klabunde,*Free Atoms, Clusters and Nanoscale Particles*,Academic Press,New York, 1994.
J. G. Verkade, *A Pictorial Approach to Molecular Bonding*, 2nd Edn, Springer-Verlag, New York, 1997.
O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
A. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, 2nd Edn, U. N. Dhur and Sons, Kolkata,2002.
I. Bertini, H. B. Gray, S. J. Lipperd and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi, 1998.
W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life,* Wiley, New York, 1994.
S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley,CA, 1993.
P. M. Harrison and R. J. Hoare, Metals in Biochemistry, Chapman and Hall, 1980.
C. A. McAuliffe (Ed) *Techniques and Topics in Bioinorganic Chemistry*, Halsted, New York, 1975.
R. W. Hay, *Bioinorganic Chemistry*, Ellis Horwood, Chichester, New York, 1984.

CH 103: Organic Chemistry

Group A

1. Stereochemistry: (18 lectures)
Chirality and symmetry, stereogenicity and stereoisomerism, stereochemical descriptors (R,S system, D,L system, E,Z system, Erythro, Threo system), Topicity relationship (homotopic, diastereotopic and enantiotopic), Topicity descriptor (*Pro-R/Pro-S, Re/Si*), determination of relative configuration: Prelog's rule, Cram's rule (Felkin modification), conformation and reactivity of monocyclic systems (3 to 8 membered rings), fused (5/5, 6/6 and 6/5), spiro and bridged bicycle systems, allylic strain, reactions of 5/6-membered ring containing one or more trigonal carbon(s)

2. Reactive intermediates with allied reaction mechanisms (18 lectures)
General methods of generation, detection, stability, reactivity and structure of the reaction intermediates: Classical and non classical carbocations and carbanions, radicals, radical cations, radical anions, carbenes, arynes and nitrenes.

Group B

3. Structure-reactivity relationship: (04 lectures)
The Hammett equation and linear free energy relationship, equilibria and rates in organic reactions, substituent and reaction constants, Taft equation.

4. Application of spectroscopy in structure elucidation: (20- 25 lectures)
Ultraviolet Spectroscopy
Theory and classification of electronic transitions, vacuum ultraviolet, Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser-Woodward rules (for conjugated dienes, carbonyl compounds), UV spectra of aromatic and heterocyclic compounds, charge transfer band.

Infrared Spectroscopy
Introduction and experimental methods, units, notation and regions; Dispersive and FT-IR,sampling techniques, complementarity of IR and Raman; fundamental vibrations, overtones, group frequencies, factors affecting group frequencies, conjugation, inductive, resonance, steric effects,application of IR in the study of hydrogen bonding, stereoisomerism, tautomerism, identification of functional groups.

NMR spectroscopy
Introduction, Magnetic properties of nuclei, Resonance condition, Field Frequency diagram,Precession of nuclei, relaxation, CW and PFT methods, sample handling, Chemical shift, Mechanism of shielding and deshielding, chemical shifts of different types of organic compounds, spin-spin coupling, germinal and vicinal coupling, Relative intensities, Chemical and magnetic equivalence of protons, protons attached to elements other than carbon, chemical exchange phenomena, temperature effects.

Mass Spectrometry and Composite Problems
Instrumentation, methods of ionization: EI, CI, Electron impact mass spectroscopy, low and high resolution, exact masses of nucleides, molecular ions, isotope ions, mass marking techniques, fragment ions of odd and even electron types, rearrangement of ions, base peak, nitrogen rule, metastable peaks, isotope peaks, isotope effects in chloro and bromo compounds, calculation of molecular formula, factors effecting cleavage patterns. Composite problems representing application of spectroscopy in structure elucidation.

Recommended Books/Journals
I.L. Finar, *Organic Chemistry*, Vol I, 6th Edn., Addison Wesley Longmann, London, 1998.
I.L. Finar, *Organic Chemistry*, Vol II, 5th Edn., ELBS, London, 1995.
J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 5th Edn., John Wiley, New York, 1999.
S. P. McManus, *Organic Reactive Intermediates*, Academic Press, New York, 1973.
F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn. Plenum Press, New York, 2001.
T. L. Gilchrist and C. W. Rees, *Carbenes, Nitrenes and Arynes*, Nelson, New York, 1973.
T. H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn. Harper and Row, New York, 1998.
W. J. I. Noble, *Highlights of Organic Chemistry*, Mercel Dekker, 1974.
E.L. Eliel, S.H. Wilen and L.N. Mander, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994. D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn., Wiley Eastern, New Delhi, 1993.
W. Kemp, *Organic Spectroscopy*, 3rd Edn., McMillan, Hong Kong, 1991.

D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5th Edn., Tata McGraw-Hill, New Delhi, 2005.
J. R. Dyer, *Applications of Absorption Spectroscopy of Organic compounds*, 2nd print Prentice_Hall,New Jersey, 1971.
R. M. Silverstein and F. Webster, *Spectrometric Identification of Organic Compounds*, 6th Edn.,John Wiley, New York, 1998.
K. Biemann, *Mass Spectrometry – Application to Organic Chemistry*, McGraw-Hill, New York,1962.
H. Budzikiewicz, C. Djerassi and D.H. Williams, *Mass Spectrometry of Organic Compounds*, Holden-Day, 1967.
R.C. Banks, E.R. Matjeka and G. Mercer, *Introductory Problems in Spectroscopy*, Benjamin/Cumings Publishing Co., 1980.
R.T. Morison, and R. N. Boyd, *Organic Chemistry*, 6th Edn., Prentice-Hall India Private Ltd., New Delhi, 1992.
J. Barker, *Mass Spectrometry*, 2nd Edn., John Wiley, New York, 2000.
K. Downard, *Mass Spectrometry*: A Foundation Course, Royal Society of Chemistry, UK, 2004.
G. Siurdek, *The Expanding Role of Mass Spectrometry in Biotechnology*, MCC Press, San diego,2004
C. Dass, *An Introduction to Biological Mass Spectrometry*, Wiley, USA, 2002.

CH 104: Physical Chemstry

Group A

1. Symmetry and group theory I: (16 lectures)
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.

2. Quantum mechanics I: (10 lectures)
Some important 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.

3. Atomic spectra: (09 lectures)
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, Paschen back effect.

Group B

4. Thermodynamics and statistical mechanics: (12 lectures)
Legendre transformation with applications; Maxwell-Boltzmann distribution with degeneracy (for both distinguishable and indistinguishable particles), partition function and its properties, interpretation of thermodynamic laws, thermodynamic function in terms of partition functions, molecular partition functions (translational, rotational, vibrational and electronic) for ideal gas, calculation of thermodynamic functions for monoatomic and diatomic gases, equipartition principle, equilibrium constant in terms of partition function.

5. Principles of molecular spectroscopy: (18 lectures)
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 nonrigidity 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.

Recommended Books/Journals
G. W. Castellan*, Physical Chemistry,* 3rd Edn, Narosa Publishing House, 1995.

I. N. Levine, *Physical Chemistry*, Tata McGraw-Hill, 1978.
G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall, India, 1997.
R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.
P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.
F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn Reprint, John Wiley and Sons, NewYork, 1999.
A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley and Sons, New York, 1998.
H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
E. Merzbacher, *Quantum Mechanics*, John Wiley and Sons, 1970.
L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, 1985.
L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1939.
C. N.Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 1994.
G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company,Tokyo, 1982.
H. E. White, *Introduction to Atomic Spectra*, McGraw-Hill Kogakusha Ltd., Tokyo, 1934.
K. Denbigh, *Principles of Chemical Equilibrium*, Cambridge University Press,Cambridge, 1981.
N. A. Gokcen and R. G. Reddy, *Thermodynamics*, Plenum Press, New York, 1996.
I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, John Wiley, New York, 1994.
F. Reif, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill, 1965.

Practical

CH 105: Inorganic Chemistry Practical

1. Experiments on quantitative estimation: analysis of mixtures, selected ores, minerals and alloys like Cr, Mn in a mixture, Dolomite, Mn in steel etc.
2. Inorganic qualitative analysis: (6 radicals including rare elements)

CH 106: Organic Chemistry Practical

1. Detection of functional groups of the supplied samples containing nitrogeneous [nitro, amide, anilide, amine (10, 20 and 30)], non-nitrogeneous (carboxylic acid, ester, aldehyde, ketone, phenolic –OH, alcoholic – OH), determination of mp / bp of the supplied sample and derivative.
Note: Samples to be given: Solid, liquid, hydrocarbon.
2. Synthesis of organic compounds involving nitration, diazotisation, photochemical reaction, Sandmayer reaction, pinacol-pinacolone rearrangement, claisen rearrangement etc.

Semester-II

Theoretical

CH 201: Analytical Chemistry

Group A

1. Separation techniques: (20 lectures)
Solvent extraction: principle, distribution ratio and partition coefficient, successive extraction and separation; different methods of extraction systems; Craig extraction and counter current distribution; problems; Chromatography: 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

2. Radiochemical methods of Analysis: (12 lectures)
Radio-analytical chemistry, Principles of G-M Counter, Proportional counter, Scintillation counter, PMT, Low level counting devices, Radiation chemistry; Radiation dosimetry- Physical dosimetry, Chemical dosimetry (Ferrous sulphate and Ceric sulphate dosimetry), Glass dosimetry. Neutron activation analysis, radioactive reagents in the analysis of trace element, organic reaction mechanisms, isotopic dilution techniques, radiometric titration.

Group B

3. Thermal methods: (14 lectures)
Different methods of analysis: TGA, DTA, DSC; thermogram, thermal stability of covalent and non-covalent bonds, thermal degradation, single crystal phase transformation, thermochemiluminescence, thermometric titration, solid state reaction kinetics.

4. Electroanalytical methods I: (18 lectures)
Electrochemical cell, electrodes: reference and indicator electrodes, membrane electrodes, electrode-solution interface layer, gas-sensing probe, ion-sensing, molecular-sensing, electrolytic process, three electrode system; electrogravimetry, coulometry, supporting electrolyte, DME; Cottrell equation, Ilkovic equation, Ilkovic-Heyrolsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, DPV, stripping voltammetry, Cyclic voltametry, amperometric titration

Recommended Books/Journals

Y. Marcus and A. S. Kertes, *Ion Exchange and Solvent Extraction of Metal Complexes*, Wiley Interscience, 1969.
H. F. Walton and W. Reiman, *Ion Exchange in Analytical Chemistry*, Pergamon Press, 1970.
A. Tarter, *Advanced Ion Chromatography*, Wiley Interscience, New York, 1989.
E. Heftman, *Chromatography*, Reinhold, New York, 1969.
G. D. Christian, *Analytical Chemistry*, 5th Edn. Wiley, New York, 1994.
J. A. Dean, *Chemical Separation Methods*, Van Nostrand Reinhold, London, 1970.
D. A. Skoog, D. M. West and F. J. Holley, *Fundamentals in Analytical Chemistry*, 5th Edn, Saunders, Philadelphia, 1988.
S. Lindsay and J. Barnes, *High Performance Liquid Chromatography*, John Wiley, New York, 1992.
D. G. Peters, J. M. Hayes and G. M. Hieftje, *Chemical Separations and Measurements: Theory and Practice of Analytical Chemistry*, Saunders, Wiley Interscience, New York, 1974.
S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, Wiley Eastern Ltd., New Delhi, 1998.
S. E. Manahan, *Environmental Chemistry*, Lewis Publishers, Boston, 1991.
J. H. Seinfeld, *Air Pollution: Physical and Chemical Fundamentals*, McGraw-Hill, New York, 1975.
R. M. Harrison (Ed), *Pollution: Causes, Effects and Control*, Royal Society of Chemistry, Great Britain, 1990.
J. E. Fergusson, *The Heavy Elements: Chemistry, Environmental Impact and Health Effects*, Pergamon Press, Oxford, 1990.
A. K. De, *Environmental Chemistry*, 4th Edn, New Age International (P) Ltd. Publications, New Delhi, 2000.
D. F. S. Natusch and P. K. Hopke, *Analytical Aspects of Environmental Chemistry*, John Wiley and Sons, New York, 1983.
O. Hutzinger (Ed.), *The Handbook of Environmental Chemistry*, Springer-Verlag, Weinheim, 1980.
W. W. Wendlandt, *Thermal Methods of Analysis*, Interscience Publishers, New York, 1964.
D. Dollimore, *General Review on Thermal Analyses*, Anal. Chem., 1994, 66, 17R.
R. C. McKenzie (Ed.), *Differential Thermal Analysis*, Academic Press, New York, 1970.

C. Duval, *Inorganic Thermogravimetric Analysis*, Elsevier Publishing Co, New York, 1963.
D. R. Crow, *Polarography of Metal Complexes*, Academic Press, London, 1979.
C. G. Zoski (Ed) *Handbook of Electrochemistry,* Elsevier, New York, 2007
A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications,* 2nd Edn.,Wiley, New York, 1998.
G. Seaborg, *Modern Alchemy*, World Scientific, 1994.

CH 202: Inorganic Chemistry

Group A

1. Chemistry of f-block elements: (16 lectures)
Terresterial abundance and distribution of lanthanides and actinides, relativistic effect, electronic configuration and oxidation states; aqueous, redox and complex chemistry in different oxidation states as applicable; electronic spectra and magnetic properties- comparison with d-block elements, Lanthanide and actinide contractions and consequences, Separation of lanthanides and actinides, Lanthanide shift reagents and uses of lanthanide compounds.

2. Structure and properties of solids: (15 lectures)
Bonding in metals: ionic, covalent and hydrogen bonded solids; perovskite, ilmenite and rutile; crystal defects, nonstoichiometric compounds; electronic properties of solids, conductors, semiconductors, insulators, superconductors; ferroelectricity, antiferroelectricity, piezoelectricity, liquid crystals-elementary idea.

Group B

3. Organometallic chemistry I: (18 lectures)
Historical development, 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. Metal-carbon bonded compounds (σ-bonded), synthesis, reactivity, oxidative addition and reductive elimination reaction, insertion reactions, Metallocycles.

4. **Chemistry of the Platinum group metals(PGMs)**: (15 lectures)
Platinum group metals: Oxidation states, valence preference toward π- donor and π-acceptor ligands, Dinitrogen complexes of Ru; Nitrosyl, carbonyl complexes of PGMs; Creutz-Taube compound, Vaska's compounds, cis platin, trans platin; Uses of PGMs in medicine and catalysts.

Recommended Books/Journals

N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn, Pergamon, New York, 1997.
G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, Prentice-Hall, New Jersey, 1999.
A. F. Holleman and E. Wifrg, *Inorganic Chemistry*, Academic Press, New York,1995.
G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
J. D. Lee, Concise *Inorganic Chemistry*, Chapman and Hall, London, 1991.
G. Wulfsberg, *Principles of Descriptive Inorganic Chemistry*, University Science Books, Mill Valley, CA, 1991.
F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*,6th Edn, John Wiley and Sons, Inc., New York, 1999.
B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn,John Wiley and Sons, Inc., New York, 2001.
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.
G. B. Richter-Addo and P. L. Legzdins, *Metal Nitrosyls*, Oxford University Press, New York, 1992.
F. A. Cotton and R. A. Walton, *Multiple Bonds Between Metal Atoms*, 2nd Edn, Clarendon Press,Oxford, UK, 1993.
D. L. Kepert, *Inorganic Stereochemistry*, Springer, Berlin, 1982.
A. von Zelewsky, *Stereochemistry of Coordination Compounds*, Wiley, New York, 1996.
S. P. Sinha, *Systematics and Properties of Lanthanides*, Riedel, Dordrecht, 1983.
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.
A. F. Wells, Structural Inorganic Chemistry, 5th Edn, Oxford University Press, Oxford, 1984.
D. M. Adams, *Inorganic Solids*, Wiley, New York, 1992.
S. R. Elliot, *The Physics and Chemistry of Solids*, John Wiley & Sons, Chichester, 1998.

W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds*, Dover Publications, New York, 1989.
M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.
T. C. W. Mak and G. –D. Zhou, *Crystallography in Modern Chemistry*, Wiley, New York, 1992.
G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 1997.
G. A. Jefferey and W. Saenger, *Hydrogen Bonding in Biological Structures*, Springer, Berlin,1991.
A. J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.
J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.
P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn, Chapman and Hall, London, 1988.
G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.
C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.
J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.

CH 203: Organic Chemistry

Group A

1. Heterocyclic chemistry: (10 lectures)
Synthesis, reactivity and uses of the following compounds and their derivatives: imidazole, pyrazole, oxazole, isooxazole, thiazole and iso-thiazole.

2. Reagents in organic synthesis: (18-20 lectures)
Hydride transfer reagents: Boron based ($NaBH_4$, $Na(CN)BH_3$, super hydride, alpine borane, selectrides etc), Aluminium based (LiAlH4 and substituted LiAlH4, Red-Al, DIBAL-H), trialkyl tin hydride, silane, diimide, enzymatic reduction (Baker's yeast). Woodward and Prevost hydroxylation, Sharpless epoxidation, PCC, PDC, Mn(IV) oxide, RuO4(TPAP), Moffat oxidation, Swern oxidation, Dess-Martin Periodinane, Peterson reaction, OsO4, 1,3- Dithiane, Wilkinson catalyst, trimethyl silyl iodide (TMSI).

3. Reactions with cyclic transition states or cyclic transition intermediates: (05 lectures)
Tethering, Robinson annulations, iodolactonization, synthesis of transfused ring, sulphur as a tether.

Group B

4. Photochemistry: (12 lectures)
Basic principles, Jablonski diagram, photosensitization and quenching, photochemistry of olefinic compounds, *cis-trans* isomerisation, Peterno-Buchi reaction, Norrish Type – I and II reactions, photoreduction of ketones, di-π methane rearrangement, photo-induced reactions in organic compounds.

5. Biomacromolecules: (15-18 lectures)
Structure of proteins: Primary, secondary, tertiary and quaternary structures; chemical and enzymatic hydrolysis of proteins, denaturation of protein. Enzymes as biological catalysts, nomenclature, classification, extraction and purification (basic concept only), Fischer's lock and key concept, Koshland's induced fit hypothesis, Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibitions of enzymes.

Recommended Books/Journals

J. A. Joule and K. Mills, *Heterocyclic Chemistry*, 4th Edition, Blackwell publishing.
R. Kartritzky, *Handbook of Heterocyclic Chemistry*, Pergamon Press, London, 1986.
J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 5th Edn., John Wiley, New York, 1999.
F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn.,
Plenum Press, New York, 2001.
I.L. Finar, *Organic Chemistry*, Vol I, 6th Edn., Addison Wesley Longmann, London, 1998.
I.L. Finar, *Organic Chemistry*, Vol II, 5th Edn., ELBS, London, 1995.
James R-Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, London, 2002.
R.S. Ward, *Selectivity in Organic Synthesis*, John Wiley & Sons, 1999, New York.
J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press,Oxford, 2001.
J.H. Fuhrhop and G. Li, Organic Synthesis, *Concepts and Methods*, Wiley VCH, New York, 2003.
R. Bruckner, *Advanced Organic Chemistry, Reaction mechanism*, Academic Press.
Michael B. Smith, *Organic synthesis*, McGraw-Hill International Editions.
W. Carruthers, I. Coldham, *Modern Methods of Organic synthesis*, 4th Edn. Cambridge.

R. Norman, J. M. Coxon, Principles of Organic Synthesis, Blackie Academic and Professional.
K. K. Rohtagi-Mukherjee, *Fundamental of Photochemistry*, Wiley-Eastern.
A. Cox, T. Camp, *Introductuctory Photochemistry*, McGraw-Hill.
R. P. Kundall, A. Gilbert, *Photochemistry*, Thomson Nelson.
J. Coxon, B. Halton, *Organic Photochemistry*, Cambridge University Press.
D. L. Nelson and M.M. Cox, *Lehninger: Principles of Biochemistry*, W.H. Freeman Co, London, 2005.
H. Neurath, *The Proteins: Composition, Structure and Function*, Vols. 1-5, Academic Press, New York, 1963.
J. P. Greenstein and M. Winitz, *Chemistry of the Amino Acids (3 Vols.)*, Wiley, New York, 1961.
H. Dugas, *Bioorganic Chemistry,* A Chemical approach to Enzyme Chemistry, 3rd Edn. Sringer International Edition.
W. J. I. Noble, *Highlights of Organic Chemistry*, Mercel Dekker, 1974.
S.W. Fox and J.F. Foster, *Introduction to Protein Chemistry*, John Wiley, New York, 1957.

CH 204: Physical Chemistry

Group A

1. Group theory II: (12 lectures)
The Great Orthogonality Theorem: statement and interpretation, proof of important corollaries; construction of character tables, cyclic groups and construction of their character tables, direct product groups and construction of their character tables, direct product representations, projection operators (without derivations) and vanishing of integrals, invariance of the Hamiltonian operator and eigenfunctions of H as bases of irreducible representations.

2. Quantum mechanics II: (12 lectures)
Degeneracy; Schrödinger equation, energy-eigenvalue equation, expectation value, eigenvalue and spread of observation, definition of uncertainty; equation of motion, constants of motion; detailed treatment of the particle in a box, including degeneracy; step potential and tunneling.

Group B

3. Electrochemistry I: (12 lectures)
Introduction, ion-solvent interaction: Born model and Born equation, enthalpy of ion solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, 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 and its importance

4. Chemical kinetics I: (12 lectures)
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 (elementary idea), dielectric effect on ion-ion reaction; electrostriction; volume of activation; effect of 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.

5. Crystal structure: (12 lectures)
Crystal symmetry: translation, glide plane and screw axis; diffraction of X-rays by crystals: Laue and Bragg conditions; concept of 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

Recommended Books/Journals

G. W. Castellan*, Physical Chemistry,* 3rd Edn, Narosa Publishing House, New Delhi, 1995.
R. A. Alberty and R. J. Silbey, *Physical Chemistry*, 1st Edn, John Wiley & Sons, Inc., 1995.
R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.
F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn Reprint, John Wiley and Sons, New York, 1999.
A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley and Sons, New York, 1998.
S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.
Volker Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi,1989.

S.N.Ghosal, *Quantum Chemistry*
F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
E. Merzbacher, *Quantum Mechanics*, John Wiley and Sons, 1970.
L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, 1985.
L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1939.
P. C. W. Davies, *Quantum Mechanics*, ELBS, 1985.
J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, London, 1961.
D. Bohm, *Quantum Theory*, Asia Pub. House, Bombay, 1960.
S. Glasstone, *An Introduction to Electrochemistry*, D. Van Nostrand Company, 1962.
J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol. I, Plenum Press, New York,1970.
K. J. Laidler, *Reaction Kkinetics,* Vols. I & II, Pergamon Press, London, 1970.
K. J. Laidler, *Chemical Kinetics,* Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.
L. P. Hammett, *Physical Organic Chemistry*, McGraw-Hill Book Company, New Delhi, 1970.
M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.
J. Albery, *Electrode Kinetics*, Oxford Chemistry Series, Clarendron Press, Oxford, 1975.
G. D. Mahan, *Many Particle Physics*, Kluer Academy, Plenum Publisher, 2000.
C. Kittel, *Introduction to Solid State Physics*, John Wiley & Sons, 4th Ed.
M. F. C. Ladd and R. A. Palmer, *Structure Determination by X-ray Crystallography*, Plenum Press,New York, 3rd Ed., 1994.
P. A. Cox, *The Electronic Structure & Chemistry of Solids*, Oxford University Press, 1987.
X. Clegg, *Crystal Structure Determination*, Oxford University Press, 2005.

Practical

CH 205: Physical Chemistry

1. Conductivity: a) Determination of strength of HCl & CH3COOH from their mixture by NaOH, b) Saponification of ester, c) Determination of CMC of micelles.
2. Potentiometry: a) Determination of E^0 of quinhydrone electrode, b) Fe2+/Fe3+ system.
3. Kinetics: a) Determination of order of reaction of I^- & BrO_3^-, b) Iodination of acetone.
4. Equilibrium: a) Determination of CST, b) Determination of coordination number of Cu^{2+}, c) Solubility product of Lead Iodide
5. Colorimetry: a) Jobś method, b) Iodination of acetone
6. Polarimetry: Study of kinetics of acid catalysed reaction of sugar.

CH 206: Analytical Chemistry & Data Processing

1. Separation techniques involving ion exchange and solvent extraction
2. Titrimetric estimation of different organic compounds
3. Data processing and elementary numerical techniques
4. Computer application in chemistry-Exposure to available standard application packages like: chemdraw, generation of graphs, data sheet creation, tables using excel programme, etc.

Semester-III

Theoretical

CH 301: Advanced General

Group A

1. Group theory III: (20 lectures)
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 ABn type and sandwitch type molecules, (iii) study of hybridization, selection rules, allowedness / forbiddenness of n-π* and π-π* 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.

2. Surface chemistry: (10 lectures)
Introduction, adsorption isotherms, surface excess; BET isotherm, LB film, membrane equilibrium, micellisation.

Group B

3. Macromolecules: (15 lectures)
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.

4. Quantum mechanics III: (15 lectures)
Exactly solvable problems: Solutions for the stationary states of harmonic oscillator (wave function and operator methods), rigid rotator and the H-atom (with complex and real solutions).

Recommended Books/Journals

S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.
F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn Reprint, John Wiley and Sons, New York, 1999.
A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley and Sons, New York, 1998.
V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York
H. -J. Butt, K. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, Wiley-VCH, 2003.
J. H. Clint, *Surface Chemistry*, Blackie and Son Ltd., 1992.
W. Adamson, *Physical Chemistry of Surfaces*, John Wiley and Sons, New York, 1990
G. S. Mishra, *Introductory Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.
C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley and Sons, Inc., New York, 1961.
F. W. Billmeyer, Text Book of Polymer Science, 2nd Edn., Wiley-Interscience, New York, 1971.
H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi,1989.
F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, London, 1961.
D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt. Ltd., New Delhi, 2003

CH 302: Advanced general

Group A

1. Metal ion promoted reactions: (14 lectures)
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, hydrosilylation, hydrophosphylation, hydroamination, hydrocyanation and hydroboration reactions, Heck reaction.

2. Molecular magnetism I: (10 lectures)
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, crsytal field diagram, high spin/low spin equilibrium.

3. Green Chemistry: (07 lectures)
Principles of Green Chemistry, Organic reactions in aqueous medium, Organic reactions using supported reagents, Solvent-free organic reactions, Micro-wave assisted organic reactions. Use of ionic liquid as recyclable reaction medium

Group B

4. Advance spectroscopic techniques: (30-35 lectures)
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; 11B, 13C, 14N, 17O, 19F and 31P-NMR : instrumentation, chemical shift and application; MS: EI,CI,FD, FAB, Plasma desorption, FAB, 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, XPS, UPS, AUGER, AES, XRF and EXAFS; Synergistic benefit: spectroscopic and other tools in structure elucidation.

Recommended Books/Journals
F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
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.
J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.
G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.
O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, II; Molecule-Based Magnets*, Wiley-VCH, Weinheim, 2001.
P. M. Lathi (Ed), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.

CH 303: Advanced general

Group A

1. Materials chemistry: (20 lectures)
Preparation of nano particles: top down and bottom up approach, electrochemical, chemical, photochemical and biochemical synthesis of nano particles. Properties of nano particles, variation of properties with size. Applications of nano particles. Synthesis and properties of carbon nanotubes. Organic conductors, liquid crystals.

2. Radiopharmaceuticals: (10 lecturers)
Nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; radionuclide generators; ideal radiopharmaceuticals, methods of radio-labelling, specific radiopharmaceuticals for diagnostic and therapeutic purposes.

Group B

3. Inorganic reaction mechanism I: (15 lectures)
Fundamentals, Mechanism of substitution reactions, water exchange, aquation, anation, acid catalysed aquation, Rate laws, Four broad classes of mechanism of substitution-Associative, Dissociative, Interchange Ia and Id; Linear free energy relationship.

4. Pericyclic Reactions I: (15-20 lectures)
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 in cycloadditions; generalised rules of pericyclic reactions.

Recommended Books/Journals

F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, 1967.
R. G. Wilkins, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
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.
F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, 1967.
R. G. Wilkins, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley and Sons, New York, 1987
R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 1998.
J. Singh and J. Singh, *Photochemistry and Pericyclic Reactions*, 2nd Edn., New Age International (P) Ltd., 2005.

CHI 304: Inorganic special

Group A

1. Synthetic methodology for transition and non-transition metal compounds: (15 lectures)
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.

2. Inorganic reaction mechanism II: (15 lectures)
Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to dn ion complexes, Experimental tests of mechanism, Base hydrolysis, Nucleophilicity parameter, Trans effect, cis effect, studies on fast reactions, Kinetics and activation parameters, Substitution without breaking the metal ligand bond, Recimization and Isomerization reactions.

Group B

3. Complexes in aqueous solution: (18 lectures)
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; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes, equilibria in biomolecular systems.

4. Supramolecular Chemistry I: (12 lecturers)
Concept and language, designing of building blocks, molecular valences, supramolecular orbitals, supramolecular arrays: ribbon, ladder, rack, braded, grid; harnessing non-covalent forces to design functional materials.

Recommended Books/Journals

L. S. Hegedus, *Transition Metal in the Synthesis of Complex Organic Molecules*, University Science Press, Mill Valley, CA, 1994.
M. Periasamy, *Organic Synthesis Using Iron-Carbonyl Reagents, Curr. Sci*., 2000, 78, (11), 1307-1313
G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.
G. R. Desiraju, *Crystal Engineering: Designing of Organic Solids*, Elsevier, New York, 1989.
F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, 1967.
R. G. Wilkins, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley and Sons, New York, 1987.

D. Benson, *Mechanism of Inorganic Reactions in Solution*, McGraw-Hill, London, 1968.
R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 1998.
J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.
A. E. Martell and R. J. Motekaitis, *Determination and use of Stability Constants,* 2nd Edn, VCH, New York, 1992.
R. M. Smith and A. F. Martell, *Critical Stability Constants*, 6 Vols, Plenum Press, New York, 1974-89.
M. Meloun, J. Havel and E. Hogfeldt, *Computation of Solution Equilibria: A Guide to Methods in Potentiometry, Extraction and Spectrophotometry*, Halsted, New York, 1988.

CHO 304: Organic special

Group A

1. Organic Synthetic Methods: (40 Lectures)
Retrosynthetic analysis; C-C bond formation reactions; ylide method, Si in C-C bond formation, organometallic; acetylides and nitriles, logistic and stereochemistry; synthesis of L-hexose (Sharpless and Masamune), synthesis of prostaglandins. Asymmetric Synthesis: The chiral pool; chiral auxiliaries, reagents and catalysts; Diels-Alder reaction, Heck reaction; alkylation of chiral enolates; dihydroxylation. Micro-wave assisted synthesis: Introduction, Background and theory, why microwave irradiation speed up chemical reactions, solvent in microwave assisted organic synthesis, microwave assisted synthesis techniques, some reactions involving alkylation, N-acylation, aromatic and nucleophilic substitution, cycloaddition, oxidation, reduction and rearrangement reactions.

Group B

2. **Organometallic chemistry and its application in organic synthesis:** (20-25 Lectures)
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 carbine Complexes.

CHP 304: (Physical Special)

Group A

1. Non-equilibrium thermodynamics: (30 lectures)
Limitations of classical (equilibrium) thermodynamics, entropy production in some simple irreversible processes, the 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 production with time, Prigogine's criterion for establishment of stationary state, applicability of Le Chateliar's principle on stationary states.

Group B

2. Photochemistry and Spectroscopy: (30 lectures)
1. Jablonski diagram, Fluorescence and phosphorescence, Delayed fluorescence, Quantum yield, Mechanism and decay kinetics of photophysical processes. Fluoresence quenching (dynamic and static), Stern-Volmer equation. Energy transfer (Forster's dipole coupling), Electron transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation phenomenon (excimer,exciplex).
2. Interaction of electromagnetic radiation with matter, Transition probabilities, Transition moment integral and its applications. Electric and magnetic dipole moments. Selection rules. Violation of Franck-Condon principle, oscillator strength. Nature of transitions (e.g., n-π*, π- π*, d-d, charge transfer) solvent effect on absorption and emission spectra, Stoke's shift.
3. Properties of electronically excited molecules: Life-time, redox potential, dipole moment, pK values. Potential energy diagram for donor acceptor system, Polarized luminescence.
4. Nonradiative intramolecular electronic transition, internal conversion, inter-system crossing. Crossing of potential energy surface (Franck-Condon factor). Adiabatic and non-adiabatic cross over. Kasha's rule.
5. Mössbauer spectroscopy: Principles, technique, chemical shift, quadruple effect, effect of magnetic field, applications.
6. NQR spectroscopy: Principle, technique, coupling in atom, applications.

Recommended Books/Journals
K. Denbigh, Thermodynamics of Steady States Katchalsky, Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, Interscience Publishers, 1967.

G. M. Burnett and A. M. North, *Transfer and Storage of Energy by Molecule*, Vol.I Wiley-Interscience, 1970.
J. N. Murrell, *The Theory of Electronic Spectra of Organic Molecules*, John Wiley and Sons, 1963.
J. B. Birks, *Photophysics of Aromatic Molecules*, Wiley-Interscience, 1969.
C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 1994.
G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill Int.Book Company, Tokyo, 1982.
I. Levine, Molecular Spectroscopy (Pearson)
G.Aruldhas, *Molecular Structure and Spectroscopy*,Prentice Hall.India
Photochemistry by J.A.Barltrop and J.D.Coyle,Wiley
J.B. Birks, *Photophysics of Aromatic molecules*, Wiley Interscience.
Raymond Chang, *Spectroscopy*.
R.P.Wayne, *Photochemistry*.
K.K. Rohatgi Mukherjee, *Fundamentals of Photochemistry*.

Practical

CHI 305: Inorganic Special Practical

1. Quantitative analysis of major and minor components in ores and alloys by gravimetric and other instrumental methods
2. Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric method.

CHI 306: Inorganic Special Practical

1. Computational Chemistry
2. Minicolumn ion-exchange separation and estimation of Ni(II), Co(II) and Fe(III)
3. Some common coordination compounds: synthesis and analysis.

CHO 305: Organic Special Practical

1. A. Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components.

CHO 306: Organic Special Practical

1. Spectroscopic analysis of organic compounds using supplied spectral data. 10marks
2. Separating techniques: Different types of chromatography including low and medium pressure condition; purification techniques: vacuum distillation and sublimation, solvent purification, crystallization. 10 marks

CHP 305: Physical Special Practical

Computer applications: Solutions of simultaneous equations: Gauss elimination, Numerical integration methods.
Potentiometric experiments**:** Determination of (i) solubility product of AgX, (ii) standard potential of Ag/Ag+, (iii) standard potential of Ag/AgX, (iv) activity coefficient of HX, (v) Potentiometric titration of halide mixture.

CHP 306: Physical Special Practical

Conductometric experiments**:** Titration of chromate/dichromate mixture, determination of CMC, Mixture of acetates, sulphate – bisulphate mixture, etc.
Numerical differentiation methods, Finite difference method to solve Schrödinger eigenvalue problem for box and oscillator.

Semester-IV

Inorganic Special

Theoretical

CHI 401

Group A

1. Supramolecular chemistry II: (15 lectures)
Definition, building block and spacer, molecular valency, supramolecular orbitals, non-covalent forces: pallet of hydrogen bondings, pi-pi and C-H…pi interactions, geometry setter, allosterism, proton and hydride sponges, principle of three C's, lock and key principle, host-guest interaction, self organization and self complementarity, receptors, superstructures in inorganic, metallo-organic, organometallic compounds, supramolecular devices.

2. Inorganic functional materials: (15 lectures)
Designed synthesis – molecules and crystals to materials; art of interweaving, predictable crystalline architecture, intermolecular and inter-ion interaction, secondary bonding, robust and directional interaction, functional materials, conducting materials, superconducting materials, non-linear optical materials, porous materials and molecular shieves, luminous materials, liquid crystals, magnetic materials, catalysts, molecular devices, nano- and mesomaterials, biomineralisations, biosensors, molecular recognitions, structure and phase transition, thermochromism, light harvesting ferroelasticity, intercalation.

Group B

3. Chemistry of Elements: (17 lectures)
Dinitrogen and dioxygen complexes of transition metals: Syntheses, structures, bonding and reactivity. Iso- and heteropolyoxometalates with respect of V, Mo and W: Syntheses, structures, reactions and uses. Syntheses, reactions, properties, structures and bonding of molybdenum blue, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red etc.

4. Diffraction study: (13 lectures)
Bravis lattices, space group and its determination, stereographic projection, techniques in X-ray structure determination, Fourier series, electron density and structure factor, methods of solving the phase problem, Patterson and direct methods for determination of crystal structures.

Recommended Books/Journals:

J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.
G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley and Sons, New York, 1987.
D. Benson, *Mechanism of Inorganic Reactions in Solution*, McGraw-Hill, London, 1968.
R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 1998.
M. F. C. Ladd and R. A. Palmer, *Structural Determination by X-ray Crystallography*, 3rd Edn, Plenum, New York, 1994.
R. C. Evans, *An Introduction to Crystal Chemistry*, 2nd Edn, Cambridge University Press, Cambridge, 1964
P. L. Huyskens and T. Zeegers-Huyskens, *Intermolecular Forces: An Introduction to Modern Methods and Results*, Springer-Verlag, Berlin, 1991.
G. A. Jeffrey, *An Introduction to Hydrogen Bonding,* Oxford University Press, Oxford, 1997.
F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.

CHI 402

Group A

1. Redox reactions and mechanism: (12 lectures)
Classifications, kinetics and mechanism, outer-sphere reaction, self-exchange rate, electron tunneling hypothesis, heteronuclear redox rection and simplified Marcus theory; Marcus cross relationship and its application, solvated electron; inner-sphere reaction, remote attack, doubly-bridged process, complementary and non-complementary redox reaction, ligand exchange, effect of bridging ligand in inner sphere reaction, intervalence electron transfer, induced reaction, electron-transport in metalloproteins.

2. Molecular magnetism II: (18 lectures)
Design and synthesis of different magnetic bodies, magnetic orbital, magnetic interactions in di- and polynuclear systems, effect of counter anion in crystal packing, cryogenic experiments, mechanisms of exchange interactions, Bleaney-Bowers equation, deliberate synthetic approach of ferromagnetically coupled systems, accidental orthogonality, canting, spin frustration, admixed-spin, spinflop, metamagnetism, long-range ordering, calculation of ground state and spin manifold, magnetization versus field studies, inorganic, organic and organometallic magnetic materials, Single-molecule-magnets.

Group B

3. Organometallic chemistry II: (20 lectures)
Design and synthesis; structure, bonding, stereochemistry, reaction and reaction pathways; nucleophilic addition and abstraction; application to organic synthesis, enantioselective functional group interconversion, chiral synthesis, protection and deprotection; transmetallation and cyclisation reactions, metallo-fullerenes, bioorganometallics, organo-lanthanoids and actinoids, organo-dendrimer, surface organometallic chemistry, Use of nontransitional metal- Tin and Zinc.

4. Inorganic Rings, Cages and Clusters: (10 lectures)
Metal-metal bonding, Low nuclearity and high nuclearity carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, caping rule, carbide, nitride, chalcogenide and halide containing metal clusters.

Recommended Books/Journals

G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd., New Delhi, 2001.
F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley and Sons, Inc., New York, 1999.
D. Katakis and G. Gordon*, Mechanisms of Inorganic Reactions*, John Wiley and Sons, New York, 1987.
D. Benson, *Mechanism of Inorganic Reactions in Solution*, McGraw-Hill, London, 1968.
R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, 1998.
J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.
A. E. Martell and R. J. Motekaitis, *Determination and use of Stability Constants,* 2nd Edn, VCH, New York, 1992.
O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, II; Molecule-Based Magnets*, Wiley-VCH, Weinheim, 2001.
P. M. Lathi (Ed), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.

CHI 403

Group A

1. Inorganic photochemistry: (15 lectures)
Photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, excimer structure, substitution, prompt and delayed reaction, decomposition, fragmentation, isomerisation, exchange and redox reactions; chemiluminescence, photochromism; selective photochemistry using laser beams; chemical actinometry, inorganic photochemistry in biological processes and their model studies; applications of photochemical reactions of coordination compounds - synthesis and catalysis, solar energy conversion and storage.

2. Advanced Bioinorganic Chemistry: (15 lectures)
Metal complexes interaction with DNA and RNA, Metal ions in genetic information carrier, Metal ions in metabolic energy transfer – mechanism of metal ion catalyzed and metal complex catalyzed non-enzymatic ATP hydrolysis.

Redox enzymes. Chemistry of iron metabolism: ferritin, transferin, siderophore and ceruloplasmin. Vitamins and Coenzymes: Vitamin B6 and B12 coenzymes, model systems.

Group B

3. Nano Science: (15 lectures)
The nano world, Physico-chemical considerations, Typical syntheses of nanoparticles, Oxide-nanotubes and fibers, Nano structure material catalysis reactions, Application of Nano-gold, Application of inorganic materials in nano field.

4. Chemistry of Uranium and Thorium: (15 lectures)
Isolation and purification of U and Th from natural sources; aqueous, redox and complex chemistry; Simple and complex U and Th compounds- preparation, structures, properties and reactions; Transuranium and transactinium elements; Nuclear reactors and atomic energy, nuclear fuel reprocessing; Indian scenario.

Recommended Books/Journals
C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
V. Balzani and V. Carassiti, *Photochemistry of Coordination Compounds,* Academic Press, New York, 1970.
A. W. Adamson and P. D. Fleischauer (Ed), *Concept of Inorganic Photochemistry,* Wiley, New York, 1975.
G. L. Geoffroy and M. S. Wrighton, *Organometallic Photochemistry*, Academic Press, New York, 1970.
B. R. Hollebone, C. H. Langford and N. Serpone, *Inorganic Photochemistry, Coord. Chem. Rev.*, 1981, 39, 181.
A. D. Kirk, *Inorganic Photochemistry, Coord. Chem. Rev.*, 1981, 39, 225.
D. Rendell and D. Mowthrope, *Fluorescence and Phosphorescence Spectroscopy*, John Wiley, New York, 1987.
E. Wayne and R. P. Wayne, *Photochemistry*, Oxford University Press, Oxford, 1996.

CHI 404

Group A

1. Luminescence, photoacoustic, Raman and flame atomic spectrometry: (18 lectures)
Molecular luminescence spectrometry - theory, instrumentation and applications; photoacoustic spectrometry; light scattering techniques including nephelometry and Raman spectroscopy flame spectrometric techniques - atomic absorption, atomic emission and atomic fluorescence, theory, instrumentation and applications of these techniques.

2. Green Chemistry: Inorganic Perspective: (12 lectures)
Basic principles of Green Chemistry and their illustrations with examples as: Prevention/Minimization of hazardous/toxic products; Designing safer chemicals - different basic approaches; Selection of appropriate auxiliary substances (solvents, separation agents etc); Designing biodegradable products; Prevention of chemical accidents.
Examples of green synthesis/reaction:
Green starting materials; Green reagents; Green solvents and reaction conditions; Green catalysis; Green synthesis-Real world cases; Biocycles, green chemistry in day to day life, principles, synthetic methods, industrial applications.

Group B

3**. Application of IR, NMR, EPR, UV-Vis, Mossbauer, ESCA etc. techniques:** (30 lectures)
Background of the spectroscopic tools, selection rules, active chemical system, elucidation of molecular structure, electronic structure, stereochemistry, bonding and reaction pathways (examples with simple and complex inorganic compounds including organomettalics and cluster compounds and bioinorganic systems).

Recommended Books/Journals
D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University press, 2001.
R. S. Drago, *Physical Methods in Inorganic chemistry*, Saunders, Philadelphia, 1977. .
A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.
H. H. Jaffe and M. Orchin, *Symmetry, Orbitals and Spectra*, Wiley, New York, 1982.
B.E.Douglas, C.A. Hollingsworth, *Symmetry in Bonding and Spectra,* , Academic press, New York, 1985.
K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compd.*, 5th Edn, Part A, Wiley,New York, 1997.

W. Henderson and J. S. McIndoe, *Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools-Techniques-Tips*, John Wiely & Sons, Ltd., Chichester, 2005.

Practical

CHI 405

1. Preparation of double salts and known coordination compounds and their analysis
2. Complexation and purification
3. Growing of single crystals
4. Elemental analyses (C, H, N and AAS)
5. Spectral, thermal, electrochemical and magnetic studies

CHI 406

Project work

1. Preparation of new inorganic and coordination compounds and their characterization Bi-, tri-, and polydentate ligands using different instrumental analysis.
2. Seminar lecture on project work/recent advanced topic

Organic Special

Theoretical

CHO 401

Group A & B

1. Biosynthetic pathways from acetate to natural products, shikimate pathways leading to various group of natural products. (13 Lectures)

2. Biomimetic synthesis of alkaloid derived from tryptophan, non-aromatic polycyclic polyketide, polyprenylated phloroglucinols and xanthones, rearrangements of complex terpenoids. (12 Lectures)

3. Chemistry of Carbohydrates: (15 lectures)
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; general treatment of polysaccharide chemistry: isolation, purification, hydrolysis, methylation and periodic oxidation, Smith degradation, Barry degradation.

4. Chemistry of Amino acids, Peptides and Nucleic acids: (25 lectures)
Amino acids and Peptides: classification, stereochemistry, synthesis and reactions; Peptides: structure determination, sequence analysis, End group analysis- N Terminus, C Terminus, Protection of amino and carboxyl group, strategy of peptide synthesis, Merrifield synthesis, structure determination. Nucleic acids: Introduction, classification, occurrence, nucleosides: isolation, properties and synthesis of ribosyl and deoxyribosyl nucleosides; biosynthesis of α-D-ribose phosphate, nucleotides: isolation, functions, structures of ribosyl and deoxyribosyl nucleotides; biosynthesis of inosinic acid, adenylic acid, guanylic acid, cytidylic acid and uridylic acid; translation and transcription (general idea), RNA and DNA (structural composition), codon, anticodon, genetic code, protein synthesis.

CHO 402

Group A

1. Pericylic Reactions II: (30 lectures)
Symmetry properties of M.O.'s, orbital symmetry conservation and Woodward-Hoffmann rule in pericyclic reaction; frontier orbital interaction, Fukui-Hoffman theory (qualitative), Dewar theory of aromatic transition state concept (qualitative); topology of cyclo-additions, periselectivity, regioselectivity, Lewis acid catalysis; solvent effect ,higher order cyclo-additions, dipolar cyclo-additions, electrocyclic reactions, sigmatropic reactions, chelotropic reaction, enereactions, selection rules.

Group B

2. Organic Photochemistry: (20 lectures)
Excited states (S1 and T1) of some photo excited organic molecules; mechanism of photo excitation; photo-induced reactivity of olefins, ketones, unsaturated ketones and various conjugated systems; photo-induced functionalisation in organic molecules involving Barton reaction, Norrish type reactions, Loeffler reaction; photo induced substitution reaction, chemiluminescence in organic reactions, Photochemical rearrangements, photo induced disproportion in aromatic systems.

3. Radical Chemistry: (15 lectures)
Basic Principles, C – C bond formation by various radical-radical and radical-nonradical coupling reactions. Synthesis of natural products. Various ring expansion, ring contraction, remote functionalisation and radical fragmentation reaction.

CHO 403

Group A

Structure elucidation and synthesis of Terpenoids (genaniol, nerol, caryophyllene, abietic acid, amyrins, lanosterol, carotenes), Steroids (nomenclature and stereochemistry, cholesterol, ergosterol, bile acids), prostaglandins. (30 Lectures)

Group B

Structure elucidation and synthesis of Alkaloids (ephedrine, nicotine, berberine, morphine, quinine, reserpine, yohimbine), Flavonoids (flavonol, isoflavones, xanthones) and Coumarins. (30 Lectures)

CHO 404

Group A

1. Medicinal Chemistry: (25 lectures)
Pharmacodynamics and pharmacokinetics Drug design and synthesis of Drugs, synthesis and chemistry of vitamins. Vitamins: Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of Vitamin A, B1, B6 and Folic acid etc.. Drugs: Introduction, classification of drugs, brief discussion of drug targets, drugs based on enzyme inhibition: Sulfa drugs, aspirin, paracetamol ; antibiotics : penicillin , chloramphenicol etc., Drug targets on nucleic acids, Definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, Concept of structure-activity relationship (SAR) and quantitative structure and relationship (QSAR).

2. Supramolecular Chemistry: (10 lectures)
From molecular to Supramolecular chemistry, non-covalent interaction. Synthetic molecular reports and their functions – crown ethers, cyclophanes, calixarenes, cyclodextrins, dendrimers etc. Supramolecular reactivity and catalysis, switching devices, molecular self assembly-supramolecular aggregates.

Group B

3. Green methodologies for organic synthesis: (12 lectures)
Twelve principles of Green Chemistry, Green synthetic methods, Organic reactions in aqueous medium, Organic reactions using supported reagents, Solvent-free organic reactions, Micro-wave assisted organic reactions with special emphasis on biologically important compounds. Use of ionic liquid, supercritical fluids and nanoparticles as catalyst.

4. Elucidation of reaction mechanism: (20 lectures)
(i) Linear free energy relationship: Hammet equation and its modifications, Separation of Inductive and Resonance effects- σI & σR scales-Taft equation-Yukawa-Tsuno equation- Elucidation of reaction mechanisms-Application of Hammett correlation to heterocyclic systems- Thermodynamic aspects of Hammett equation- Dual substituents parameter (DSP) Dual substituents parameter-nonlinear resonance (DSP-NLR) correlations- Taft-Bromilow-Brownlee approach.
(ii) Application of Tracer in studying reaction mechanism with special reference to carbocation and carbanion chemistry.

Practical

CHO 405

1. A. Multistep synthesis of organic compounds
B. Isolation of some common natural products

CHO 406

1. Project / Review work 30 marks
2. Seminar Lecture 20 marks.

Physical Special

Theoretical

CHP 401

Group A

1. Chemical Kinetics II: (18 lectures)
Introduction, autocatalysis, chain reactions: branched and non-branched kinetic rate equations, Semenov treatment for branched chain reactions; explosion: population explosion, upper and lower ignition/explosion limits; thermal ignition and ignition temperature; chemical oscillation: some models (Lotka, Oregonater and Brusselator); analysis of Lotka and Brusselator model, conditions for oscillation, chemistry of BZ reaction (Brusselator model).

2. Non-ideal systems: (12 lectures)
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.

Group B

3. Quantum chemistry I: (30 lectures)
Antisymmetry of many electron wave function, spin and spatial orbitals. Example of He atom and the independent particle model. Hartree vs. Hartree-Fock method. Slater determinant. Coulomb and exchange integrals with their properties; vertical ionization potential and Koopman's theorem; variational solution of the closed-shell wave function — formulation of the Hartree-Fock equations, properties of Hartree-Fock operator and wave functions, discussion of electron correlation.

Hückel theory and its underlying approximations: Hückel wave functions and aromaticity, use of SALC. Theories of valence: VB and MO theories with emphasis on the nature of functions and their properties. The H_2^+ and H_2 problem.

CHP 402

Group A

1. Approximate Quantum-mechanical methods: (20 lectures)
Variation method: Variation theorem, application to ground states of different systems, extension to excited states, linear variation, Matrix mechanics; eigenvalues-eigenvectors and diagonalisation. Perturbation Theory: Time independent formalism: Rayleigh-Schrödinger theory of non-degenerate systems, degenerate perturbation theory, Stark effect. Time dependent formalism: Transition probability, Fermi golden rule, Einstein transition probabilities, spontaneous and induced emission.

2. Biophysical Chemistry (10 Lectures)
Introduction: The cell and its constituents, proteins, nucleic acids, RNA and DNA, enzymes etc., molecular basis of life. Bioenergetics and Thermodynamics: Molecular interpretation of Energy and Enthalpy, Non-covalent reactions, hydrophobic interactions, Protein and Nucleic Acids. Biochemical Applications of thermodynamics, Thermodynamics of Metabolism, Role of ATP in biological Systems (hydrolysis of ATP).
Biological Membranes, Membrane Equilibrium, Transport through cell membrane, Active and Passive Transport, Osmosis and Diffusion, Muscle Contraction, Energy Generation.

Group B

3. Spectroscopy: (18 lectures)
Transition between states, selection rules and forbidden transitions; NMR: Relaxation and exchange phenomena, theories of chemical shift and nuclear spin-spin coupling in 2-spin systems with applications, pulsed NMR (spin echo). Electronic: n-π*, π- π* and CT transitions; vibrational: simple polyatomic molecules, normal modes,

influence of nuclear spin on vibration-rotation spectra of polyatomics; Raman: classical and quantum treatment of rotational and vibrational Raman spectra, polarization and depolarization of Raman lines, resonance Raman spectroscopy.

4. Angular momentum: (12 lectures)
Angular momentum operators, their commutation properties, step-up and step-down operators, Eigen-ket ladder and formulation of spherical harmonics from angular momentum rules, spin angular momentum, Pauli spin matrices — spin eigenfunctions and their properties, application to single electron and multi-electron atom.

Recommended Books/Journals
C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn, Tata McGraw-Hill Publishing
Company Ltd., New Delhi, 1994.
G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company, Tokyo, 1982.
A. E. Derome, *Modern NMR Techniques in Chemical Research*, Pergamon Press, Oxford, 1987.
W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, 1986.
J. K. M. Sanders, E. C. Constable and B. K. Hunter, *Modern NMR Spectroscopy: A Workbook of Chemical Problems*,
Oxford University Press, Oxford, 1993.
H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.
P. Hendra, C. Jones and G. Warnes, *FT-Raman Spectroscopy*, Ellis-Harwood, 1991.
K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 5th Edn, Part B, John Wiley and Sons, Inc., New York, 1997.
A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
E. Merzbacher, *Quantum Mechanics*, John Wiley and Sons, 1970.
L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, 1985.
L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1939.
I. N. Levine, Quantum Chemistry, 4th Edn., Prentice Hall of India Pvt. Ltd., New Delhi, 1995
J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, 1961.
D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt. Ltd., New Delhi, 2003
G. C. Schatz and M. A. Ratner, *Quantum Mechanics in Chemistry*, Dover Publication, Inc, New York, 2002.
H. L. Strauss, *Quantum Mechanics*, Eastern Economy Edition, Prentice Hall of India Pvt. Ltd., New Delhi.

CHP 403

Group A

1. Statistical Mechanics: (30 lectures)
Microcanonical, canonical and grand canonical ensembles, statistical distribution and properties of distribution function, the H theorem and approach to equilibrium; Maxwell-Boltzmann (MB), Bose-Einstein (BE) and Fermi-Dirac (FD) distributions, the derivation of thermodynamic relations, thermodynamic and characteristic features of MB, BE and FD systems (ideal cases), black body radiation and photon gas; applications: (i) statistical thermodynamics of ideal systems (effect of nuclear spin and electronic angular momentum), (ii) specific heat of solids — Debye treatment, (iii) non-ideal gas.

Group B

2. Electric and magnetic properties of matter: (16 lectures)
Dielectric polarization; Debye equation and its limitation; Onsager's reaction field model; electric polarizability of molecules; magnetic susceptibility — diamagnetic and paramagnetic, Courie law.

3. Molecular interactions: (14 lectures)
Hamiltonian in absence and presence of external fields, forces in molecules, Hellmann-Feynmann theorem, perturbative treatment of electric polarisability, intermolecular interaction — calculation of dispersion energy, the London formula.

Recommended Books/Journals
F. Reif, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill, 1965.
S. K. Ma, *Statistical Mechanics*, World Sci., 1985.

E. S. R. Gopal, *Statistical Mechanics and Properties of Matter*, Ellis Horwood, England, 1974.
R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 1996.
F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
D. W. Davies, The Electric and Magnetic Properties of Molecules.
A. J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.
C. J. F. Böttcher, Theory of Electric Polarisation, Elsevier Scientific Publishing Co., New York, 1973 (Vol. 1 & 2).

CHP 404: Physical Special

Group A

1. Catalysis: (20 lectures)
Fundamentals of adsorption and catalysis**:** Physical and Chemical adsorption – adsorption isotherms: evaluation, chemisorption on metals and metal oxides. Catalysis: concept of activity, selectivity, poisoning, promotion and deactivation. Types of catalysis: homogeneous, heterogeneous. Heterogeneous catalysis and catalytic kinetics: concept of Langmuir-Hinshelwood
Preparation and Characterization of Catalyst: general methods for preparation of catalysts: precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation of catalysts: calcinations, reduction. Catalyst characterization: surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FT-IR and thermal methods.
Nanomaterials and Catalysis: General definition, Nanochemistry basics, distinction between molecules, nanoparticles and bulk materials. Physico-chemical considerations of nanomaterials. Size-dependent properties.
Catalysis in green chemistry and environmental applications**:** Purification of exhaust gases from different sources: auto-exhaust catalysts (petrol vehicles, diesel vehicles), VOC removal; ozone decomposition; photocatalysis in effluent treatment.
Photo-catalysis**:** Photoprocesses at metals, oxides and semiconductors: concepts and mechanism. Photocatalysis application in organic pollutant degradation present in water and air.
Application of Heterogeneous catalysis: Food industry, fine chemicals, petroleum industry, petrochemical industry, heavy inorganic chemicals, catalysis in atmospheric pollution (at least one example of application should be discussed).

2. Polymer Chemistry: (10 lectures)
Configuration of polymer chains. Crystal structure of polymers. Crystallization and melting. The glassy state and the glass transition. Solid Polymer electrolytes (SPE). Block copolymers. Polymer colloids. Inter-penetrating network (IPN) polymers, Biomedical polymers.

Group B

3. Chemical Kinetics III: (20 lectures)
Unimolecular reactions: Lindemann, Hinshelwood and RRK theory. Absolute rate theory, Expression for rates in terms of atomic and molecular partition functions. Study of fast reactions - flow process and relaxation techniques, and their implementation.

4. Electrochemistry II: (10 lectures)
Debye-Huckel Theory, Debye-Huckel-Onsager Theory; electrophoretic and relaxation effects; Wien effect and Debye- Fulkenhagen effects. Helmholtz, Guoy-Chapman and Stern double-layer models.

Recommended Books/Journals

W. Adamson, Physical Chemistry of Surfaces, Wiley Intersciences, 1990 (5^{th} edition) 1990.
Bond, G C**,** Heterogeneous Catalysis: Principles and Application. Oxford University Press 1987
D.K. Chakrabarty and B. Viswanathan, Hetergogeneous Catalysis, Hardcover - Oct 2008 New Age International Publishers)
B.C. Gates, Catalytic Chemistry, John Wiley and Sons Inc. (1992).
G. Cao, Nanostructures and Nanomaterials - Synthesis, Properties and Applications, World-Scientific, 2004.
P.T. Anastas and J.C.Warner, Green Chemistry, theory and practice,
Nick Serpone and Ezio Pelizzetti, Photocatalysis: Fundamentals and Applications, Wiley, NewYork, NY, 1989.
Heterogeneous catalysis principles and application, G.C.Bond.
Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)
Catalysis: Principles and Applications, B.Vishwanathan, S. Sivasankar and A.V.Ramaswamy (Narosa Pub. House, New Delhi, 2004)

Advanced material in catalysis, James J. Burton and Robert L.Garten, Academic press, New York, 1977.
F.W. Billmeyer, Jr., Text Book of Polymer Science, 3rd edition (1984), Wiley Interscience, New York.
G. Odien, Principles of Polymerization, 3rd edition (1991) John Wiley & Sons, Singapore.
P. Bahadur and N.V. Sastry, Principles of Polymer Science, (2002) Narosa, New Delhi.
A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
E. Merzbacher, *Quantum Mechanics*, John Wiley and Sons, 1970.
L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, 1985.
L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1939.
I. N. Levine, Quantum Chemistry, 4th Edn., Prentice Hall of India Pvt. Ltd., New Delhi, 1995
S P. C. W. Davies, *Quantum Mechanics*, ELBS, 1985.
J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, 1961.
S. Glasstone, *An Introduction to Electrochemistry*, D. Van Nostrand Company, 1962.
J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol. I, Plenum Press, New York,1970.
K. J. Laidler*, Reaction Kkinetics,* Vols. I & II, Pergamon Press, London, 1970.
K. J. Laidler*, Chemical Kinetics,* Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.
M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.
P. C. Jordan, *Chemical Kinetics and Transport*, John Wiley and Sons, Inc., 1979.
M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford University Press, 1995

Practical

CHP 405: Physical Practical

Kinetic experiments: Activation energy, effect of solvent dielectric constant, effect of ionic strength.
Spectrophotometric experiments: determination of pK_{in}, salt effect, solvent effect and micellar effect on rate.
Phase diagram of ternary mixtures.

CHP 406: Physical Practical

Project Work: 30 marks
Seminar lecture on project work/any advanced topics: 20 marks