

DRAFT SYLLABUS

for

M. Sc. Course in

Chemistry

To be effective from the session 2007-09



THE UNIVERSITY OF BURDWAN

BURDWAN 713 104

WEST BENGAL, INDIA

THE UNIVERSITY OF BURDWAN

Syllabus for M. Sc. Course in Chemistry
Distribution of papers and marks

(A) SEMESTER-I

THEORETICAL

Paper*	Division	Marks	Lect. Hrs.	Exam. Hrs.
CG 101	A + B	45	54	3
CG 102	A + B	45	54	3
CG 103	A + B	45	54	3
CG 104	A + B	45	54	3
Internal assessment		20**		
Subtotal:		200		

*General paper

**Each paper with 5 marks for internal assessment

PRACTICAL

Paper	Division [¶]	Marks	Lab. Hrs.	Exam. Hrs.
CGP 105	15 + 10 + 25	50	50	5
CGP 106	-Do-	50	50	5
Subtotal:		100		

[¶]15 sessional, 10 viva, 25 examination

Total of Semester-I (Theory + Practical): 300 Marks

(B) SEMESTER-II

THEORETICAL

Paper*	Division	Marks	Lect. Hrs.	Exam. Hrs.
CG 201	A + B	45	54	3
CG 202	A + B	45	54	3
CG 203	A + B	45	54	3
CG 204	A + B	45	54	3
Internal assessment		20**		
Subtotal:		200		

*General paper

**Each paper with 5 marks for internal assessment

PRACTICAL

Paper	Division [¶]	Marks	Lab. Hrs.	Exam. Hrs.
CGP 205	15 + 10 + 25	50	50	5
CGP 206	-Do-	50	50	5
Subtotal:		100		

[¶]15 sessional, 10 viva, 25 examination

Total of Semester-II (Theory + Practical): 300 Marks

(C)

SEMESTER-III

THEORETICAL

Paper ^{¶¶}	Division	Marks	Lect. Hrs.	Exam. Hrs.
CAG 301	A + B	45	54	3
CAG 302	A + B	45	54	3
CAG 303	A + B	45	54	3
CS 304	A + B	45	54	3
Internal assessment		20**		
Subtotal:		200		

^{¶¶}Papers CAG 301, CAG 302 and CAG 303 (advanced general) common to all and Paper CS 304 to respective specials

** Each paper with 5 marks for internal assessment

PRACTICAL

Paper ^{¶¶}	Division [¶]	Marks	Lab. Hrs.	Exam. Hrs.
CGP 305	15 + 10 + 25	50	50	5
CSP 306	-Do-	50	50	5
Subtotal:		100		

[¶]15 sessional, 10 viva, 25 examination

^{¶¶}Paper CGP 305 common to all and Paper CSP 306 to respective specials

Total of Semester-III (Theory + Practical): 300 Marks

(D) SEMESTER-IV

THEORETICAL

Paper ^{¶¶}	Division	Marks	Lect. Hrs.	Exam. Hrs.
CAG 401	A + B	45	54	3
CS 402	A + B	45	54	3
CS 403	A + B	45	54	3
Internal assessment		15**		
Subtotal:		150		

^{¶¶}Paper CAG 401 (advanced general) common to all and Papers CS 402 and CS 403 to respective specials

**each paper with 5 marks for internal assessment

PRACTICAL

Paper ^{¶¶}	Division	Marks	Lab. Hrs.	Exam. Hrs.
CSP 404	50 [§]	50	50	5
CCA 405	50 [§]	50	50	5
CTP 406 ^{§§}	35 + 10 + 5 ^{§§§}	50	50	-
Subtotal:		150		

^{¶¶}Paper CSP 404 to respective specials and Paper CCA 405 (computer application in chemistry) and CTP 406 (term paper) common to all

[§]15 sessional, 10 viva, 25 examination

^{§§}Focusing contents of Papers CS 402 and CS403

^{§§§}35 For preparation of term papers, 10 seminar, 5 viva

Total of Semester-IV (Theory + Practical): 300 Marks

Grand Total (Semester-I + Semester-II + Semester-III + Semester-IV): 1200 Marks

Semester-I
Theoretical
CG 101: Inorganic General
Group A

1. Valency theories — quantum chemical approach: (13 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 H_n type systems, isolobal analogy

2. Coordination chemistry — bonding, stereochemistry and structure: (14 lectures)

Crystal field theory, crystal field diagram, ligand field theory, molecular orbital theory and angular overlap model; spectral properties, vibronic coupling, intensity stealing, band broadening, spectrochemical series, nephelauxetic series; magnetic properties; structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibria

Group B

3. Cluster compounds: (13 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, chevreton compounds, infinite metal chains, cluster-surface analogy.

4. Bioinorganic chemistry: (14 lectures)

Metal ions in biology, myoglobin, hemoglobin, hemocyanin, hemerythrin, cytochromes, rubredoxin, ferredoxins; biological fixation of nitrogen, chlorophyll and photosynthesis; PS-I, PS-II, 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, metallothionein, xanthine oxidase,

sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; vitamin B₁₂ and B₁₂-enzyme; toxicity and detoxification of metal ions; chelation therapy.

Tentative List of 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. Lippard 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.

CG 102: Nuclear-Analytical General**Group A**

1. Nuclear properties and structure: (22 lectures)

Fundamentals, mass-energy relationship, nuclear binding energy and its role in nuclear stability, concept of nuclear angular momentum, magnetic dipole moment and electronic quadrupole moment (elementary idea), parity of nuclear energy states; liquid drop model, 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

2. Statistics of radioactivity measurements: (05 lectures)

Statistical models, application of counting statistics in nuclear measurements

Group B

3. Radioactive equilibrium: (08 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

4. Cosmochemistry: (04 lectures)

Different geological systems, age of rocks and earth, cosmic rays and its effect in meteorites, nuclear reactions in stars

5. Nuclear detection techniques and spectroscopy: (15 lectures)

Principle of nuclear detection, gas detector, ionization chamber, proportional and G. M. detector, dead time of detectors; Mossbauer spectroscopy: Mossbauer effect — conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds, NQR

Tentative List of Recommended Books/Journals

- H. J. Arnika, *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. Ramamoorthy, *Fundamentals of Radiochemistry*, Yancas, Mumbai, 2004
- V. I. Goldanskii and R. H. Herber, *Chemical Applications of Mossbauer Spectroscopy*, 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.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.

CG 103: Organic General

Group A

1. Stereochemistry: (20 lectures)
- Molecular symmetry and chirality; stereoisomerism: definitions, classifications; configuration and conformation; relative and absolute configuration; determination of relative configuration: Prelog's rule, Cram's rule (Felkin modification), and Sharpless rule; conformations of acyclic and cyclic system (3 to 8 membered rings), fused (5/5 & 6/6), spiro and bridged bicyclo systems; stability, reactivity and mechanism; allylic strain; reactions of 5/6-membered ring containing one or more trigonal carbon(s)
2. Quantitative relationship between structure and reactivity: (07 lectures)
- Linear free energy relations: Hammett equation; equilibria and rates in organic reactions; separation of polar, steric and resonance effects: Taft equation, Grunwald - Winstein equation

Group B

3. Application of spectroscopy in structural elucidation: (27 lectures)

Ultraviolet Spectroscopy

Transitions, vacuum ultraviolet, applications in conjugated dienes, some correlation studies, trienes, polyenes, steroids and triterpenoids, stereochemical applications, α,β -unsaturated carbonyl compounds; solvent effect, applications in aromatic and heterocyclic compounds (05 lectures)

Infrared Spectroscopy

Concept of vibrational spectra, stretching and bending vibrations, application identification of functional groups, applications in sequence of organic synthetic reactions and in the structure elucidation of simple organic molecules, FTIR (06 lectures)

NMR spectroscopy

Chemical shift, coupling constant and application in organic molecules

(06 lectures)

Mass Spectrometry

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 ions, factors affecting cleavage patterns

(10 lectures)

Tentative List of Recommended Books/Journals

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.

W. J. I. Noble, *Highlights of Organic Chemistry*, Merceel 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.

CG 104: Physical General

Group A

1. Symmetry and group theory I: (09 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: (09 lectures)

Summarization of the results of some experiments — black-body radiation, photoelectric effect, Davison and Germer experiment, Franck-Hertz experiment, Young's double slit experiment; identification of classical and quantum systems, Bohr's correspondence principle with examples; postulates of quantum mechanics, properties of wave functions, operators and related theorems

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, Paschenback 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: (15 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 non-rigidity on spectral features; vibrational spectra of diatomics: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: origin; selection rules; P, Q and R branches; Raman spectra: origin, selection rules, rotational and vibrational Raman spectra of diatomics; NMR spectra: theory, relaxation process, instrumentation, chemical shift and shielding, factors contributing to magnitude of shielding, spin interactions — its origin, equivalent protons, qualitative idea of energy levels of AX and A₂ systems, a few representative examples

Tentative List of 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, New York, 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

CGP 105: Inorganic General

1. Experiments on quantitative estimation: analysis of selected ores, minerals and alloys
2. Synthesis and characterization of inorganic and coordination compounds: selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands

CGP 106: Nuclear-Analytical General

1. Radioactivity measurements
2. Separation techniques involving ion exchange and solvent extraction
3. Titrimetric estimation of different organic compounds
4. Beer's law: application in different chemical matrices

Semester-II

Theoretical

CG 201: Inorganic General

Group A

1. Chemistry of elements — comparative accounts: (27 lectures)
Design and synthesis, geometric and electronic structures, stereochemistry and bonding, reactivity and reaction pathways of various coordination compounds of

transition and non-transition metal ions with halide, pseudohalide, aquo, hydroxo, oxo, carboxylate, amine, amide, polypyridine, azoimine, phosphine, carbonyl, nitrosyl, dioxolene, azophenol, macrocycle, Schiff base etc. and their mixed mono-, bi-, and polynuclear complexes; a closer look at the applications of coordination molecules in different fields of chemistry and related disciplines

Group B

2. Structure and properties of solids: (18 lectures)

Bonding in metals, ionic, covalent and hydrogen bonded solids; perovskite, ilmenite and rutile; spinel and inverse spinel, silicates: pyroxene, amphibole, talc, mica, clay, zeolite, ultramarine; crystal defects, non-stoichiometric compounds; electronic properties of solids, conductors, semiconductors, insulators, superconductors; ferroelectricity, antiferroelectricity, piezoelectricity, liquid crystals, cooperative magnetism

3. Organometallic chemistry I: (09 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

Tentative List of 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. Wifrig, *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. Jeffrey 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.

CG 202: Nuclear-Analytical General

Group A

1. Separation techniques: (18 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. Environmental chemistry: (09 lectures)

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 and their chemical speciation; eutrophication, waste water treatment — primary, secondary and tertiary treatment nuclear waste; nuclear accidents, control of air pollution: different methods — gravitational settling chamber, cyclone separators, electrostatic precipitation; role of plants, various sources of soil pollution; noise pollution: classification, hazards

Group B

3. Thermal methods: (09 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: (12 lectures)

Electrochemical cell, electrodes: reference and indicator electrodes, membrane electrodes, electrode-solution interface layer, gas-sensing probe, electrolytic process, three electrode system; supporting electrolyte, DME; Cottrell equation, Ilkovic equation, Ilkovic-Heyroslsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, stripping voltammetry, amperometric titration

5. Synthetic elements: (06 lectures)

Man made elements: theoretical background, production and separation with special reference to actinoids and superheavy elements, solution chemistry in terms of electronic configuration

Tentative List of 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.

CG 203: Organic General

Group A

1. Reactive intermediates with allied organic reaction mechanism: (15 lectures)
 Classical and non-classical carbocations and carbanions; radicals, radical cations, radical anions, carbenes, arynes and nitrenes; general methods of generation, detection, stability, reactivity and structure of the intermediates; olefin metathesis
2. Carbohydrate chemistry: (12 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

Group B

1. Heterocyclic chemistry: (09 lectures)

Synthesis, reactivity and uses of the following compounds and their derivatives: imidazole, pyrazole, oxazole, iso-oxazole, thiazole and iso-thiazole

2. Protein chemistry: (18 lectures)

Classification (according to their composition, shapes or structures, nutrition, function of essential amino acids); evaluation of protein quality: biological value, digestibility co-efficient, PER and NPU; peptide bond, Pauling's studies and conclusion on peptide bond, denaturation of proteins, factors effecting denaturation, essential criteria for structure elucidation of protein; primary structure, solubility studies, amino acid analysis, molecular weight determinations (chemical method, ultracentrifugation, gel-filtration, gel-electrophoresis), C-terminal and N-terminal amino acid determinations, secondary, tertiary and quaternary structures, factors responsible for stabilization of secondary and tertiary structures, Merrifield's solid state peptide synthesis

Tentative List of Recommended Books/Journals

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.

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.

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.

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.

E. A. Davidson, *Carbohydrate Chemistry*, Holt, Rinehart and Winston, New York, 1967.

R. D. Guthrie and J. Honeyman, *An Introduction of Chemistry of Carbohydrate*, 3rd Edn., Clarendon Press, Oxford, 1988.

J. Kennedy, *Carbohydrate Chemistry*, Clarendon Press, Oxford, 1988.

A.R. Kartiritzky, *Handbook of Heterocyclic Chemistry*, Pergamon Press, 1986.

K. Nakanishi, T. Goto, S. Ito, S. Natori and S. Nozoe, *Natural Products Chemistry*, Vol. I, Academic Press, New York, 1974.

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. Kartritzky, *Handbook of Heterocyclic Chemistry*, Pergamon Press, London, 1986.

CG 204: Physical General

Group A

1. Group theory II: (09 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: (09 lectures)

Degeneracy; Schrödinger equation, energy-eigenvalue equation, expectation value, eigenvalue and spread of observation, definition of uncertainty; equation of motion, constants of motion; exactly solvable problems: harmonic oscillator, rigid rotator, step potential and tunneling; elementary discussion of the H-atom solution

3. Electrochemistry: (09 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

Group B

4. Chemical kinetics: (12 lectures)

Theories of reaction rates: applications to uni-, bi- and termolecular 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; study of fast reactions — flow process and relaxation techniques

5. Crystal structure: (15 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

Tentative List of 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.
 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 Kinetics*, 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, Clarendon Press, Oxford, 1975.
 G. D. Mahan, *Many Particle Physics*, Kluwer 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

CGP 205: Organic General

1. Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components
2. Synthesis of organic compounds involving important chemical reactions (nitration, diazotisation, Beckmann transformation, photochemical reaction, Sandmeyer reaction, pinacol-pinacolone rearrangement)

CGP 206: Physical General

1. Experiments in kinetics
2. Experiments in equilibrium
3. Instrumental methods: potentiometry, polarimetry, colorimetry and conductometry
4. Data processing and elementary numerical techniques

Semester-III

Theoretical

CAG 301: Advanced General

Group A

1. Group theory III: (18 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 AB_n type and sandwich type molecules, (iii) study of hybridization, selection rules, allowedness/forbiddenness of $n-\pi^*$ and $\pi-\pi^*$ transitions, (iv) splitting of terms in octahedral and tetrahedral ligand fields, Orgel and Tanabe-Sugano diagrams, (v) symmetry aspects of molecular vibrations — infrared and Raman activity, conservation of orbital symmetry in pericyclic reactions

2. Surface chemistry (09 lectures)

Introduction, adsorption isotherms, surface excess; BET isotherm, LB film, membrane equilibrium, micellisation

Group B

3. Macromolecules: (12 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. Advanced spectroscopic methods: (15 lectures)

Instrumentation, presentation of spectra, active chemical system; INDOR, COSY, NOESY in ^1H NMR; functional group characterization, fluxionality, distortion and dynamic equilibria; long-range spin-spin interaction; ^{11}B , ^{13}C , ^{14}N , ^{17}O , ^{19}F and ^{31}P -NMR: instrumentation, chemical shift and application; EI, CI, FD, FAB-Mass, MALDI-TOF; isotropic effect, fragmentation patterns and application in structure elucidation; CD/ORD: methods, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application; EPR: anisotropy, intensity, hyperfine splittin, Kramer's theorem, photoelectron spectroscopy, ESCA, UPS, Auger, AES, XRF and EXFAS; Synergistic benefit: spectroscopic and other tools in structure elucidation

List of Recommended Books/Journals

- 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.
- V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
- W. Adamson, *Physical Chemistry of Surfaces*, John Wiley and Sons, New York, 1990
- 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.
- G. S. Mishra, *Introductory Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.
- G. W. Castellan, *Physical Chemistry*, 3rd Edn., Narosa Publishing House, 1995.
- R. A. Alberty and R. J. Silbey, *Physical Chemistry*, 1st Edn., John Wiley and Sons, Inc., New York, 1995.
- P. Ghosh, *Polymer Science and Technology of Plastic and Rubber*, Tata McGraw-Hill Publishing Company Limited, New Delhi, 1993.
- C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley and Sons, Inc., New York, 1961.
- I. N. Levine, *Physical Chemistry*, 4th Edn., Tata McGraw-Hill, New Delhi, 1995.

- S. F. Sun, *Physical Chemistry of Macromolecules: Basic Principles and Issues*, John Wiley & Sons, New York, 1994.
- F. W. Billmeyer, *Text Book of Polymer Science*, 2nd Edn., Wiley-Interscience, New York, 1971.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- J. G. Grasselli, M. K. Snavely and B. J. Bulkin, *Chemical Application of Raman Spectroscopy*, Wiley, New York, 1981.
- 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.
- W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, 1986.
- H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.
- N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.
- L. Kevan and R. N. Schwartz (Eds), *Time Domain Electron Spin Resonance*, John Wiley, New York, 1979.
- J. E. Wertz and J. R. Boulton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman and Hall, London, 1986.
- D. W. Turner, C. Baker and C. R. Bundle, *Molecular Photoelectron Spectroscopy*, Wiley Interscience, New York, 1970.
- J. H. D Eland, *Photoelectron Spectra*, Butterworth, London, 1984.
- T. L. Barr, *Modern ESCA: the Principles and Practice of X-ray Photoelectron Spectroscopy*, CRC Press, Boca Raton, 1994.
- D. P. Woodruff and T. A. Delchar, *Modern Techniques of Surface Science*, Cambridge University Press, Cambridge, 1988.
- T. Thomson, M. D. Baker, A. Christie and J. F. Tyson, *Auger Electron Spectroscopy*, John Wiley, 1985.

CAG 302: Advanced general Group A

1. Metal ion promoted reactions: (12 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, hydrosilation, hydrophosphilylation, hydroamination, hydrocyanation and hydroboration reactions, Heck reaction
2. Electroanalytical methods II: (10 lectures)
- Cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV; methods, choice of solvent, supporting electrolyte, working

electrode, switching potential, electrode potential, pathways of electron transfer: EEE, ECE; electro-induced reactions; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn, ZEBRA system

3. Radiopharmaceuticals: (05 lecturers)

Nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; radionuclide generators; ideal radiopharmaceuticals, methods of radiolabelling, specific radiopharmaceuticals for diagnostic and therapeutic purposes

Group B

3. Complexes in aqueous solution: (09 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. Reaction mechanism: (09 lectures)

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

5. Molecular magnetism I: (09 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, crystal field diagram, high spin/low spin equilibrium

Tentative List of 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.

G. Wulfsberg, *Principles of Descriptive Inorganic Chemistry*, University Science Books, Mill Valley, CA, 1991.

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.
- J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.
- G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.
- C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.
- 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.
- R. M. Smith and A. F. Martell, *Critical Stability Constants*, 6 Vols, Plenum Press, New York, 1974-89.
- A. E. Martell and R. J. Motekaitis, *Determination and use of Stability Constants*, 2nd Edn, VCH, New York, 1992.
- M. Meloun, J. Havel and E. Hogfeldt, *Computation of Solution Equilibria: A Guide to Methods in Potentiometry, Extraction and Spectrophotometry*, Halsted, New York, 1988.
- 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.
- C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.
- 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.

CAG 303: Advanced General

Group A

1. Photochemistry: (12 lectures)
Photochemical energy, Jablonski diagram, photosensitisation and quenching, Norrish type-I and type-II processes, Paterno-Buchi reaction, photochemistry of unsaturated compounds: rearrangement of unsaturated compounds; photo-induced reactions in aromatic compounds
2. Pericyclic Reaction: (09 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, periselectivity in cycloadditions; generalised rules of pericyclic reactions

3. Reaction with cyclic transition states or cyclic intermediates: (06 lectures)

Tethering, Robinson annulations, iodolactonisation; synthesis of transfused ring; sulfur as a tether

Group B

3. Reagents in organic synthesis: (18 lectures)

Hydride transfer reagent: Boranes, trialkyl borohydrides, Diimide, Baker's yeast, trialkyl tin hydride; DIBAL, Na(CN)BH₃, Woodward and Prevost hydroxylation, Sharpless epoxidation, PCC, PDC, Mn(IV) oxide, RuO₄ (TPAP), Moffat oxidation, Swern oxidation, Dess-Martin Periodinane; Shapiro reaction, Peterson reaction, OsO₄, SeO₂

3. Enzyme chemistry and metalloproteins: (09 lectures)

Introduction, classification, formation and function of enzymes, co-enzymes, cofactors (elementary idea); Metalloproteins: Composition and functions of Haemoglobin, Hemocyanin, Ceruplasmin, Ferritin and Cytochrome 'C'

Tentative List of Recommended Books/Journals

T.L.Gilchrist and R.C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn., Cambridge University Press, 1979.

R.B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.

T.H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn., Harper and Row, 1998.

I. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, John Wiley, 1980.

W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn., Low Price Edition, Cambridge University Press, 1996.

H. O. House, *Modern Synthetic Reactions*, 2nd Edn., Benjamin, 1971

J. Singh and J. Singh, *Photochemistry and Pericyclic Reactions*, 2nd Edn., New Age International (P) Ltd., 2005

CS 304: Inorganic special

Group A

1. Synthetic methodology for transition and non-transition metal compounds:

(12 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: (15 lectures)

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, inorganic nucleophilicity scales; Edward scale, n_{pt} scale, Gutmann donor number, Drago E & C scale, trans effect, cis effect, reactions without metal-ligand bond breaking, water exchange rates, proton ambiguity, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters - tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand; reactions in fluxional organometallic compounds

Group B

3. Application of IR, NMR, EPR, UV-Vis, Mossbauer, ESCA etc. techniques:

(27 lectures)

Background of the spectroscopic tools, selection rules, active chemical system, elucidation of molecular structure, electronic structure, stereochemistry, bonding and reaction pathways in halide, pseudohalide, carbonyl, nitrosyl, DMSO, phosphine, polypyridine, azopyridine, oxime, quinone, macrocyclic (porphyrin, phthalocyanine) and organometallic (acetyl acetonate, azobenzene, cyclopentadienyl anion, allyl, allene, carbocyclic) metal complexes; enumeration and characterization: geometrical (*cis/trans*, *fac/mer*) and stereo (optical) isomers in different polyhedra; Jahn-Teller distortion, effective π -acceptance centre, ligational motif and chelate loop, electron-transfer site, μ -bonding and hapticity, acidity/basicity of coordinate molecule, electrophilicity/nucleophilicity, quasi-aromaticity and super-aromaticity, fluxionality, metalloligand, probing reaction centre, reactivity and reaction pathways (intramolecular/intermolecular, stereoretentivity/stereodynamicity), evaluating Hammett

and Taft parameters, assignment of d-d, MLCT, LMCT, LLCT, IVCT transitions, covalency of ML bonding in coordination complexes

Tentative List of 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.
- N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn, Pergamon, New York, 1997.
- 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. Wilkinns, *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.
- C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.
- G. Aruldas, *Molecular Structure and Spectroscopy*, 2nd Edn., Prentice-Hall of India, New Delhi, 2007.
- D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University press, 2001.
- R. S. Drago, *Physical Methods in Inorganic chemistry*, Saunders, Philadelphia, 1977.
- C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
- A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.
- D. N. Sathyanarayana, *Vibrational Spectroscopy Theory and Applications*, New Age International, New Delhi, 1996.
- H. H. Jaffe and M. Orchin, *Symmetry, Orbitals and Spectra*, Wiley, New York, 1982.
- B. E. Douglas and C. A. Hollingsworth, *Symmetry in Bonding and Spectra, An Introduction*, Academic press, New York, 1985.
- K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 5th. Edn, Part A, Wiley, New York, 1997.
- B. Schrader (Ed.) *Infrared and Raman Spectroscopy: Methods and Applications*, VCH Weinheim, 1995.
- W. Henderson and J. S. McIndoe, *Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds: Tools-Techniques-Tips*, John Wiely & Sons, Ltd., Chichester, 2005.
- 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.
- A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal Ions*, Clarendon Press, Oxford, 1970.
- N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.
- W. O. George and H. O. Willis, *Computer Methods in Ultraviolet, Visible and Infra-red Spectroscopy*, Royal Society of Chemistry, 1990.
- E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, *Structural Methods in Inorganic Chemistry*, 2nd Edn., Blackwell Scientific Publications, Oxford, 1991.
- F. Gerson, *High Resolution ESR. Spectroscopy*, John Wiley, New York, 1971.
- L. Kevan and R. N. Schwartz (Eds), *Time Domain Electron Spin Resonance*, John Wiley, New York, 1979.
- J. E. Wertz and J. R. Boulton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman and Hall, London, 1986.

CS 304: Nuclear-Analytical Special

Group A

1. Theory of radioactive decay: (10 lectures)
 Introduction, quantum mechanical aspects of radioactive disintegration, alpha decay paradox and its explanation in terms of tunnel effect, Geiger-Muller relationship, time-dependant perturbation theory, Golden rule and its application in explaining beta and gamma transition, selection rules
2. Nuclear force and structures: (17 lectures)
 Two body problem — properties of deuteron and derivation of depth-range relationship, its applications in explaining nature of nuclear force, elementary particles; nuclear models — strong and weak interaction, nuclear magnetic dipole moment and electric quadruple moment in terms of shell model, collective model, Fermi gas model, nuclear excitation, idea of nuclear temperature and entropy

Group B

3. Nuclear reaction: (10 lectures)
 General features, types of nuclear reaction, conservation laws, nuclear reaction dynamics, mechanism of nuclear reaction, use of uncertainty principle, resonance and non-resonance reaction, optical model and calculation of mean free path, nuclear fission and fusion reaction, calculation of fission probability from Bohr-Wheeler's theory

4. Detectors: (12 lectures)

Proportional detectors: proportional counter performance, gas multiplication factor, space charge effects, resolution, time characteristics of signal pulse; scintillation detectors: different types, pulse shape analysis, resolution and detection efficiency, liquid scintillation detectors; semiconductor detector: general characterization, depletion depth, resolution and efficiency, pulse rise time, surface barrier detector; some basic ideas of pulse processing and shaping, single- and multi-channel analysers

5. Coincidence counting (05 lectures)

Determination of absolute disintegration rates, decay scheme studies

List of Recommended Books/Journals

- G. Friedlander, E. F. Macias, J. W. Kennedy and J. M. Miller, *Nuclear and Radiochemistry*, Wiley Interscience, New York, 1981.
- I. Kaplan, *Nuclear Physics*, Addison-Wesley, Cambridge, 1963.
- R. D. Evans, *The atomic nucleus*, McGraw-Hill, New York, 1979.
- G. F. Knoll, *Radiation Detection and Measurements*, John Wiley and Sons, New York, 1979.
- W. R. Leo, *Techniques of nuclear and particle physics experiments*, Narosa Publishing House, 1995.
- S. S. Kapoor and V. S. Ramamurthy, *Nuclear Radiation Detections*, New Age International, New Delhi, 1986
- H. J. Arnikar, *Essentials of Nuclear Chemistry*, New Age International, 4th Edn, New Delhi, 2001.
- H. J. Arnikar, *Nuclear Chemistry through Problems*, 4th Edn, New Age International, 1995.
- S. B. Patel, *Nuclear Physics*, New Age International, New Delhi, 1996.
- G. Choppin, J. O. Lilienzin and J. Rydberg, *Radiochemistry and Nuclear Chemistry*, Butterworth-Heinemann, 2001.
- B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice-Hall, 1965.
- B. L. Cohen, *Concepts of Nuclear Physics*, McGraw-Hill, New York, 1971.
- M. Haissinsky, *Nuclear Chemistry Audits Application*, Addison Wesley, 1965.
- R. Eisberg and R. Resnick, *Quantum Physics of Atoms, Molecules, Nuclei and Particles*, 2nd Edn, John Wiley and Sons, New York, 1985.
- M. Lefort, *Nuclear Chemistry*, D. Van Nostrand, London, 1968.
- L. R. B. Elton, *Nuclear Sizes*, Oxford University Press, 1961.
- D. Holliday, *Introductory Nuclear Physics*, Wiley, New York, 1955.
- G. M. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, Wiley, New York, 1955.
- J. M. Blatt, V. F. Weissleopf, *Theoretical Nuclear Physics*, Wiley, New York, 1952.

CS 304: Organic Special Group A

1. Organometallic chemistry: (12 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 carbyne complexes

2. Terpenes: (08 lectures)

Structural studies on sesquiterpenes, diterpenes, triterpenes and carotenoids; chemistry of carryophyllene, abietic acid, β -amyirin, α and β -carotenoids

3. ^{13}C NMR spectrometry: (07 lectures)

Introduction, theory, instrumentation, chemical shifts, coupling constants, application in organic molecule characterization

Group B

5. Stereo selective reactions of alkenes and carbonyl compounds: (18 lectures)

Nucleophilic addition: use of chiral substrates, auxiliaries, reagents and catalysts; asymmetric conjugate addition; addition of allyl boron derivative; reactions at alpha carbon: enolate formation (regioselectivity and stereoselectivity); stereoselective enolate alkylation (oxazolidinone, oxazoline); aldol reaction, asymmetric aldol reaction; hydroboration, hydrogenation, dihydroxylation, cyclopropanation, epoxidation

6. ORD-CD: (09 lectures)

Introduction, theory, cotton effect curves and applications, octant rule, axial haloketo rule, lactone sector rule

Tentative List of Recommended Books/Journals:

T.H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn., Harper and Row, 1998.

J. March, *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 5th Edn., John Wiley, 1999.

F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4th Edn., Plenum Press, 2001.

K.C. Nicolson and E.J. Sorensen, *Classics in Total Synthesis*, VCH, 1996.

P. Deslongchamps, *Stereoelectronic Effect in Organic Chemistry*, Pergamon Press, 1983.

R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd Edn., ELBS, 2003..

W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn., Low Price Edition, Cambridge University Press, 1996.

- S. Hanessain, *Total Synthesis of Natural Products : The Chiron Approach*, Pergamon Press, 1984.
- K. Nakanishi, T Goto, Sho Ito, S. Natori, and S. Nozoe, *Natural Products Chemistry, Vol. I* (1974) and *Vol. II* (1975), Academic Press.
- K.J. Hale, *The Chemical Synthesis of Natural Products*, Sheffield Academic Press/CRC Press, 2000.
- I. L. Finar, *Organic Chemistry, Vol. II*, 5th Edn., ELBS, 1995.
- P. De Mayo, *The Higher Terpenoids*, Interscience Publishers, 1959.
- A. R. Pinder, *The Chemistry of Terpenes*, Chapman and Hall, 1960.
- F. Hill, *Organotransition Metal Chemistry*, Royal Society of Chemistry, 2002.
- J. Pearson, *Metalloorganic Chemistry*, 1985.
- R. H. Crabtree, *The Organometallic Chemistry of Transition Metals*, 2nd Edn., John Wiley, 1994.
- E. Abel, F.G.A. Stone and G. Wilkinson, *Comprehensive Organometallic Chemistry*, Vols. 3-10, Pergamon Press, 1980-1995.
- A. Yamamoto, *Organo-Transition Metal Chemistry*, John Wiley, 1986.
- J. Tsujiz, *Organic Synthesis by Means of Transition Metal Complexes*, Springer-Verlag, 1975.
- G. Davies, *Organo Transition Metal Chemistry : Application in Organic Synthesis*, Pergamon Press, 1982.
- J. P. Collman and S. L. Hegedus, *Principles and Applications of Organo-Transition Metal Chemistry*, University Science Book, 1986.
- R. C. Mehrotra and A. Singh, *Organometallic Chemistry : A Unified Approach*, 2nd Edn., New Age International Pvt. Ltd., New Delhi, 2000.
- R. M. Acheson, *Introduction of Chemistry of Heterocyclic Compounds*, 2nd Edn., Interscience Publisher, 1967.
- R. Kartritzky, *Handbook of Heterocyclic Chemistry*, 1st Print, Pergamon Press, 1986.
- E. Breitmaier and W. Voelter, *¹³C NMR Spectroscopy : Methods and Application in Organic Chemistry*, 3rd Edn., Verlag Chemie, 1987.
- R. S. Word, *Selectivity in Organic Synthesis*, John Wiley & Sons.
- J. R. Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, 2002.
- E.M. Carreira, O. Rerser, *Classics in Stereoselective Synthesis*, John Wiley & Sons, 2007.
- R. S. Atkinson, *Stereoselective Synthesis*, Wiley, 1995.
- C. Bolm, J. A. Gladysz, *Chemical Reviews* 2003, 103 (8).
- T. D. W. Claridge, *Tetrahedron Organic Chemistry Series Volume 19, High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, 2004.
- M. Duer (Ed), *Introduction to Solid State NMR Spectroscopy*, Blackwell, 2004.

CS 304: Physical Special

Group A

1. Thermodynamics of irreversible processes: (15 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 Chatelier's principle on stationary states

2. Kinetics: (12 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, Oregonator and Brusselator); analysis of Lotka and Brusselator model, conditions for oscillation, chemistry of BZ reaction (Brusselator model); theories of unimolecular reactions: Lindemann, Hinshelwood and RRK theory

Group B

3. Mathematical methods: (09 lectures)

Elementary vector calculus, equation of continuity of fluid motion, diagonalisation of square symmetric matrices (real elements) by Jacobi method; coordinate transformation — the Jacobian and its use

4. Non-ideal systems: (09 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

2. Photochemistry: (09 lectures)

Production of excited states, singlet and triplet states, spin-orbit coupling, radiative and non-radiative processes, fluorescence and phosphorescence: mirror image relationship, quantum yield, life-time and anisotropy; properties of excited states: dipole moment, pK_a , energy transfer, quenching, excimers and exciplexes, special photochemical reactions, flash photolysis, laser flash photolysis

List of Recommended Books/Journals

- I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, Interscience Publishers, 1967.
- V. N. Kondrat'ev, *Chemical Kinetics of Gas Reactions*, Pergamon Press, 1964.
- 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.
- M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.
- S. K. Scott, *Oscillations, Waves, and Chaos in Chemical Kinetics*, Oxford University Press, 1994.
- E. N. Yeregin, *The Foundation of Chemical Kinetics*, Mir Publishers, 1979.
- K. J. Laidler, *Chemical Kinetics*, TMH Publishing Company Limited, 1988.
- E. Kreyszig, *Advanced Engineering Mathematics*, 5th Edn., Wiley Eastern, 1988.
- G. Arfken, *Mathematical Methods for Physicists*, Academic Press, New York, 1966.
- M. K. Jain, *Numerical Methods for Scientific and Engineering Computation*, Wiley Eastern Ltd.
- R. A. McQuarrie and J. D. Simons, *Physical Chemistry* 1st Edn, Viva Books Private Limited, New Delhi, 1998.
- R. A. McQuarrie, *Statistical Mechanics*, Harper and Row, 1976.
- L. D. Landall and E. M. Lifshitz, *Statistical Physics* 2nd revised English Edn., Pergamon Press, Oxford, 1977.
- J. N. Murrell, *The Theory of Electronic Spectra of Organic Molecules*, John Wiley and Sons, 1963.
- J. B. Burks, *Photophysics of Aromatic Molecules*, Wiley-Interscience, 1969.
- G. M. Burnett and A. M. North, *Transfer and Storage of Energy by Molecule*, Vol. I, Wiley-Interscience, 1970

Practical

CGP 305: Inorganic, Nuclear-Analytical, Organic and Physical General

Inorganic

1. Solution electrical conductivity measurements, and spectral, thermal, electrochemical and magnetic studies of coordination compounds

Nuclear-Analytical

2. Spectrophotometric analysis of binary mixtures, and determination of indicator constant
3. Determination of water quality parameters

Organic

4. Spectrophotometric identification of simple organic compounds (IR, and UV-Vis)

Physical

5. Experiments on kinetics-I: effect of solvent, pH, ionic strength

CSP 306: Inorganic Special

1. Quantitative analysis of major and minor components in ores and alloys by volumetric, complexometric, gravimetric and other instrumental methods after separation of the components by solvent extraction or chromatographic techniques
2. Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric methods

CSP 306: Nuclear-Analytical Special

1. Quantitative analysis of major, minor and trace components of ores and alloys by conventional and instrumental methods like spectrophotometer and AAS
2. Analysis of water, cement, fertilizer, food and drug
3. Experiments on separation techniques by ion exchange chromatography and solvent extraction processes

CSP 306: Organic Special

1. Different types of chromatography including low and medium pressure condition; purification techniques: vacuum distillation and sublimation, solvent purification, crystallization,
2. Quantitative estimation of organic compounds

CSP 306: Physical Special

1. Experiments on surface chemistry: determination of CMC by conductometric, tensiometric, viscometric and spectrophotometric methods
2. Experiments on kinetics-II: variable temperature, experiments on equilibrium, micelles

Semester-IV
Theoretical
CAG 401: Advanced General
Group A

1. Diffraction study: (12 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

2. Supramolecular Chemistry I: (06 lectures)

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

3. Luminescence, photoacoustic, Raman and flame atomic spectrometry: (09 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

Group B

4. Quantum chemistry: (14 lectures)

Legendre, associated Legendre polynomials; Hermite polynomials; Lagurre and associated Lagurre polynomials; polynomials as orthonormal functions, their properties; complete solution of the H-atom problem; angular momentum: operators, their commutation properties, step-up and step-down operators, application to single electron and multi-electron atom, eigen-ket-ladder and formulation of spherical harmonics from angular momentum rules, finite rotation operation vs. angular momentum operators, spin angular momentum, Pauli spin matrices — spin eigenfunctions and their properties

5. Spectroscopy: (13 lectures)

Maxwell's field equations, 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: $n\text{-}\pi^*$, $\pi\text{-}\pi^*$ 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

Tentative List of Recommended Books/Journals

- 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.
- W. E. Addison, *Structural Principles in Inorganic Compounds*, John Wiley, New York, 1961.
- 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.
- G. A. Jeffrey and W. Saenger, *Hydrogen bonding in Biological Structures*, Springer, Berlin, 1991.
- S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape*, Elsevier, Amsterdam, 1997.
- F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.
- B. Dietrich, P. Viout and J. -M. Lehn, *Macrocyclic Chemistry – Aspects of Organic and Inorganic Supramolecular Chemistry*, VCH, Weinheim, 1993.
- J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.
- G. R. Newkome, C. N. Moorefield and F. Vogtle, *Dendritic Molecules*, VCH, Weinheim, 1996.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.
- 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.
- 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.
- 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. 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.
 A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal Ions*, Clarendon Press, Oxford, 1970.
 N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.
 W. O. George and H. O. Willis, *Computer Methods in Ultraviolet, Visible and Infra-red Spectroscopy*, Royal Society of Chemistry, 1990.

CS 402: Inorganic special

Group A

1. Electrochemical studies: (18 lectures)

Preamble, switching and action potentials, electrode potential and factors affecting; cyclic voltammetry, differential pulse voltammetry and coulometry; reversible, quasireversible and irreversible processes; E, EE, ECE, EC, ECEC paths, protic-electroprotic equilibria; electroinduced reactions — electrosynthesis, electrocatalysis, electropolymerisation, electrocrystallisation, electrochemiluminescence; OTTLE, surface-modified electrode, photoelectrochemistry, spectroelectrochemistry, excimer and its structure, excited state potential, redox orbital, redox series, redox isomer, electron hopping, spacially isolated orbitals; conjunctive study and simulations of electron transfer sites

2. Redox reactions: (09 lectures)

Classifications, kinetics and mechanism, outer-sphere reaction, self-exchange rate, electron tunneling hypothesis, heteronuclear redox reaction 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

Group B

3. 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

4. Organometallic chemistry II: (12 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

Tentative List of Recommended Books/Journals

- P. W. Atkins, *Physical Chemistry*, 5th Edn., Oxford University Press, Oxford, 1994.
 D. I. G. Ives and G. J. Janz, *Reference Electrodes*, Academic Press, New York, 1961.
 J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Plenum Press, New York, 1970.
 D. T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr., *Experimental Electrochemistry for Chemists*, 2nd Edn, Wiley, New York, 1995.
 S. R. Morrison, *Electrochemistry in Semiconductor and Oxidised Metal Electrodes*, Plenum Press, New York, 1980.
 J. Koryta and K. Stulik, *Ion-selective Electrodes*, Cambridge University Press, Cambridge, 1983.
 A. J. Bard, R. Parsons and J. Jordan, *Standard Potentials in Aqueous Solution*, Dekker, New York, 1985.
 S. Torii, *Electro-Organic Syntheses*, Part I: *Oxidations*, Part II: *Reductions*, VCH, Weinheim, 1985.
 A. J. Fry and W. E. Britton (Eds.), *Organic Electrochemistry*, Dekker, New York, 1985.
 E. Heitz and G. Kreysa, *Principles of Electrochemical Engineering*, VCH, Weinheim, 1986.
 D. E. Kyriacou and D. A. Jannakoudis, *Electrocatalysis for Organic Synthesis*, Wiley, New York, 1986.
 J. Goodisman, *Electrochemistry: Theoretical Foundations*, Wiley, New York, 1987.

- A. P. F. Turner, I. Karube and G. S. Wilson (Ed.), *Biosensors: Fundamentals and Applications*, Oxford University Press, Oxford, 1987.
- R. J. Gale (Ed.), *Spectroelectrochemistry: Theory and Practice*, Plenum Press, New York, 1988.
- M. I. Ismail (Ed.), *Electrochemical Reactors: Their Science and Technology*, Elsevier, Amsterdam, 1989.
- J. Janata, *Principles of Chemical Sensors*, Plenum Press, New York, 1989.
- D. Pletcher and F. C. Walsh, *Industrial Electrochemistry*, 2nd Edn., Chapman and Hall, London, 1990.
- R. Varma and J. R. Selman (Eds.), *Techniques for Characterization of Electrodes and Electrochemical Processes*, Wiley, New York, 1991.
- J. Koryta, *Ions, Electrodes, and Membranes*, Wiley, Chichester, 1991.
- J. O'M. Bockris and S. U. M. Khan, *Surface Electrochemistry*, Plenum Press, New York, 1993.
- C. M. A. Brett and A. M. O. Brett, *Electrochemistry: Principles, Methods and Applications*, Oxford University Press, Oxford, 1993.
- K. V. Kordesch, *Fuel Cells and Their Applications*, VCH, Weinheim, 1994.
- P. A. Christensen and A. Hammett, *Techniques and Mechanisms in Electrochemistry*, Blackie, Edinburgh, 1995.
- P. G. Bruce, *Solid-state Electrochemistry*, Cambridge University Press, Cambridge, 1995.
- F. Goodrich and K. Scott, *Electrochemical Process Engineering*, Plenum Press, New York, 1995.
- W. Schmickler, *Interfacial Electrochemistry*, Oxford University Press, Oxford, 1996.
- C. A. Vincent and B. Scrosati, *Modern Batteries*, 2nd Edn., Arnold, London, 1997.
- C. H. Hamann, A. Hammett and W. Vielstich, *Electrochemistry*, Wiley-VCH, New York, 1998.
- A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications*, 2nd Edn, Wiley, New York, 1998.
- H. Taube, *Electron Transfer Reaction of Complex Ions in Solution*, Academic Press, New York, 1970.
- A. Haim, *Inner-Sphere Reactions*, Progr. Inorg. Chem, 1983, 30, 273.
- N. Sutin, *Outer-Sphere Reactions*, Progr Inorg Chem. 1983. 30, 441.
- W. L. Reynolds and R. W. Lumry, *Mechanism of Electron Transfer*, Ronald Press, New York, 1966.
- C. J. Ballhausen, *Introduction to Ligand Field Theory*, McGraw-Hill, New York, 1962.
- A. N. Figgis, *Introduction to Ligand Field Theory*, Interscience, New York, 1966.
- S. C. Rakshit, *Molecular Symmetry Groups and Chemistry*, The New Book Stall, Kolkata, 1988.
- 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.
- J. P. Collmann, L. S. Hegehus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransition metal Chemistry*, University Science Books, Mill Valley, CA, 1987.
- E. Abel, F. G. A. Stone and G. Wilkinson (Eds.) *Comprehensive Organometallic Chemistry*, Vols. 1-8, Pergamon Press, Oxford 1980-1995.

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

R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 2nd Edn, Wiley, New York, 1994.

G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, Prentice-Hall, New Jersey, 1997.

A. Yamamoto, *Organotransition Metal Chemistry*, Wiley, New York, 1986.

CS 402: Nuclear-Analytical Special

Group A

1. Chemistry of exotic atoms and hot atom chemistry: (09 lectures)

Positron annihilation, probability of positronium formation, reaction and mechanism of positronium ion, chemistry of muonium and pionium ions; hot atom chemistry, Szilard-Chalmer reaction and retention of activity, primary and secondary retention, synthesis of labelled compounds

2. Applications of radiotracers: (18 lectures)

Isotope dilution; DIDA, IIDA and substoichiometric methods of analysis, application and numerical problems; nuclear activation analysis: principles, classifications and methods of nuclear activation analysis: principle, different types, interferences, K_0 methods and comparative methods for analysis, special types of derivative activation analysis, depth profile activation analysis, cyclic activation analysis, secondary particle activation analysis; problems and applications, charged-particle activation analysis (CPAA): principles, calculation, applications, PGNA, PIXE, PIGE, IPAA, RBS; design of a new radiopharmaceutical: general considerations and factors; biosynthesis, factors in labeling: efficiency, isotope effect, storage conditions, radiolysis; specific methods of labeling; quality control; physicochemical and biological test

Group B

3. Chemical and biological effects of radiation: (15 lectures)

Ionizing radiation and its physical and chemical effect in target, water, radiolysis, (definition of different units in radiation chemistry, calculation of radiation dose, biological effects, source of human data, lethal dose, permissible level of radiation dose), primary radiological products of water and their characterization, dosimetric concepts and quantities,

different types of chemical dosimeters, thermoluminescence and lyoluminescence and explanation — different unusual reactions by lyoluminescence

4. Nuclear reactor and accelerators: (12 lectures)

General features and types of reactor, four-factor formula, charge particle accelerator, van de Graff generator, linear accelerator, cyclotron, synchrotron, synchrocyclotron

List of Recommended Books/Journals

- J. Green and J. Lee, *Positronium Chemistry*, Academic Press, 1964.
 J. Turner, *Atoms, Radiation and Radiation Protection*, Willey Interscience, 1995.
 S. Ahrland, J. O. Liljerzin and J. Rydberg, *Chemistry of the Actinides*, Pergamon Press, 1986.
 J. J. Katz, G. T. Seaborg, L. R. Morss (Ed), *Chemistry of the Actinide Elements*, Chapman and Hall, London, 1986.
 W. D. Ehmann and D. E. Vance, *Radiochemistry and Nuclear Methods of Analysis*, John Wiley, 1991.
 J. W. T. Spinks and R. J. Woods, *An Introduction to Radiation Chemistry*, Wiley, New York, 1964.
 J. F. Duncan and G. B. Cook. *Isotopes in Chemistry*, Clarendon Press, Oxford, 1968.
 I. M. Kolthoff, P. J. Elving and E. B. Sandell, *Treatise on Analytical Chemistry*, Pt-I, II, III, The Interscience Encyclopedia, Inc., New York. 1959,
 A. I. Vogel, *A Text Book of Quantitative Inorganic Analysis*, 3rd Edn, Longmans, 1961.

CS 402: Organic Special

Group A

1. Organic Photochemistry: (15 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; photochemical rearrangements, photo induced disproportion reaction, photo induced substitution reaction in aromatic systems, chemiluminescence in organic reactions

2. Alkaloids: (12 lectures)

Classification, general reactions of alkaloids, typical reactions, conversions and rearrangements of morphine, papaverine and cinchona alkaloids

Group B

4. Organic synthetic process: (15 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 (Sharplaeess and Masamune), synthesis of prostaglandins

5. Spectroscopy and stereochemistry: (12 Lectures)

NMR; 3J variation with dihedral angle, fused rings, spreading out effect, vicinal coupling in other ring sizes, geminal coupling; shapes of NMR signals, pi contribution, NOE; 2D-NMR, EI-MS, MALDI-TOF-MS

Tentative List of Recommended Books/Journals

- G.J. Calvert and J.N. Pitts, *Photochemistry*, 2nd Print, John Wiley, New York, 1967.
 N. J. Turro, *Molecular Photochemistry*, Benjamin and Co., 1955.
 O.L. Chapman, *Some Aspects of Organic Photochemistry*, Dekker, 1967.
 W.A. Noyes, G.S. Hammond and J.N. Pitts, *Advances in Photochemistry*, Vol. I Interscience Publisher, 1964.
- P. de Mayo, *Organic Photochemistry*, IUPAC, Butterworths, London, 1960.
 J.M. Coxon and B. Halton, *Organic Photochemistry*, Cambridge University Press, Cambridge, 1974.
 C.H.J. Wells, *Introduction to M.L. Photochemistry*, Chapman and Hall, 1974.
 D.C. Neekers, *Mechanistic Organic Photochemistry*, Reinhold, 1967.
 T.L. Gilchrist and R.C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn., Cambridge University Press, 1979.
 R.B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.
 R. Streitwieser, *Molecular Orbital Theory of Organic Chemists*, John Wiley, 1961.
 R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley, 1994.
 K.C. Nicolson and E.J. Sorensen, *Classics in Total Synthesis*, VCH, 1996.
 W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn., Low Price Edition, Cambridge University Press, 1996.
 R.S. Ward, *Selectivity in Organic Synthesis*, John Wiley & Sons., 2003
 K. Nakanishi, T Goto, Sho Ito, S. Natori, and S. Nozoe, *Natural Products Chemistry, Vol. I* (1974) and Vol. II (1975), Academic Press.
 K. W. Bentley, *The Alkaoids, Part II*, Interscience Publishers, 1965.
 S.W. Pelletier, *Chemistry of the Alkaloids*, Van Nostrand Reinhold Co., 1970.
 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.
 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.
- H. Budzikiewicz, C. Djerassi and D.H. Williams, *Structure Elucidation of Natural Products by Mass Spectrometry*, Vol. I and Vol. II, Holden-Day, 1964.
- N. S. Bhacca, S. Norman and D. H. Williams, *Application of NMR Spectroscopy in Organic Chemistry*, Holden-Day, 1964.
- R.B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.
- 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.
- R. S. Word, *Selectivity in Organic Synthesis*, John Wiley & Sons.
- J. R. Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, 2002.
- E.M. Carreira, O. Renser, *Classics in Stereoselective Synthesis*, John Wiley & Sons, 2007.
- R. S. Atkinson, *Stereoselective Synthesis*, Wiley, 1995.
- C. Bolm, J. A. Gladysz, *Chemical Reviews* 2003, 103 (8).
- T. D. W. Claridge, *Tetrahedron Organic Chemistry Series Volume 19, High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, 2004.
- M. Duer (Ed), *Introduction to Solid State NMR Spectroscopy*, Blackwell, 2004.
- F. Hillenkamp, J. P. Katalinic, *A Practical Guide to MALDI MS: Instrumentation, Method and Applications*, 2006.

CS 402: Physical Special

Group A

1. Statistical mechanics: (27 lectures)

Classical equations of motion: Newton, Lagrange and Hamilton's forms, Poisson Bracket in classical mechanics, relation of Poisson Bracket's with commutators in quantum mechanics, phase space, Liouville's equation and theorem, 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: (12 lectures)

Dielectric polarization; Debye equation and its limitation; Onsager's reaction field model; electric polarizability of molecules; magnetic susceptibility — diamagnetic and paramagnetic, Curie law

3. Molecular interactions: (15 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

Tentative List Recommended of Books/Journals

- E. S. R. Gopal, *Statistical Mechanics and Properties of Matter*, Ellis Horwood, England, 1974.
 R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 1996.
 F. Reif, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill, 1965.
 S. K. Ma, *Statistical Mechanics*, World Sci., 1985.
 F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, 1990.
 P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
 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).
 D. W. Davies, *The Electric and Magnetic Properties of Molecules*,

CS 403: Inorganic Special

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, allostereism, 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 materials: (12 lectures)

Designed synthesis – molecules and crystals to materials; art of interweaving, predictable crystalline architecture, intermolecular and interion interaction, secondary bonding, robust and directional interaction, functional materials, conducting materials,

superconducting materials, non-linear optical materials, porous materials and molecular sieves, 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. 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

4. Correlative study: (09 lectures)

Thermodynamic and kinetic parameters; diagnostic tools: spectroscopic, electrochemical, thermal, magnetic, crystallographic tools; parameters: stretching frequency, chemical shift, potential value, bond distance, bond angle and torsion angle, magnetic moment value, Mossbauer shift value, rate constant, half life, dissociation constant, correlation diagram, room temperature and variable temperature results

Tentative List of Recommended Books/Journals:

- J. E. Mark, H. R. Allcock and R. West, *Inorganic Polymers*, Prentice Hall, Englewood Cliffs, New Jersey, 1992.
- D. W. Bruce and D. O'Hare, *Inorganic Materials*, John Wiley and Sons, New York, 1992.
- R. B. King (Ed), *Encyclopedia of Inorganic Chemistry*, Wiley, Chichester, 1994.
- Special issue on Focus on Self-assembly, *Acc. Chem. Res.*, 1999, 32, Number 4.
- 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.
- G. A. Jeffrey and W. Saenger, *Hydrogen bonding in Biological Structures*, Springer, Berlin, 1991.
- S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape*, Elsevier, Amsterdam, 1997.
- F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.
- B. Dietrich, P. Viout and J. -M. Lehn, *Macrocyclic Chemistry – Aspects of Organic and Inorganic Supramolecular Chemistry*, VCH, Weinheim, 1993.

- J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.
- G. R. Newkome, C. N. Moorefield and F. Vogtle, *Dendritic Molecules*, VCH, Weinheim, 1996.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, John Wiley and Sons, New York, 2000.
- V. Balzani and F. Scandola, *Supramolecular Photochemistry*, Ellis Horwood, Chichester, 1991.
- F. L. Caster, R. E. Siatowski and H. Woltzen (Eds.), *Molecular Electronic Devices*, North Holland, Amsterdam, 1999.
- D. J. Williams (Ed.), *Nonlinear Optical Properties of Organic and Polymeric Materials*, ACS, Washington DC, 1983.
- S. R. Marder, J. E. Sohn and G. D. Stucky (Eds.), *Materials for Non-linear Optics: Chemical Perspectives*, ACS Symposium Ser, 1991.
- R. W. Boyd, *Nonlinear Optics*, Academic Press, San Diego, 1992.
- R. L. Carlin, *Magnetochemistry*, Springer-Verlag, New York, 1986.
- 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. Day and A. E. Underhill (Eds.), *Metal-organic and Organic Molecular Magnets*, RSC, London, 2000.
- P. M. Lathi (Ed.), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.
- C. M. Sorensen, *Magnetism in Nanoscale Materials in Chemistry*, Wiley Interscience, New York, 2001.
- S. Chandrasekhar, *Liquid Crystals*, 2nd Edn, Cambridge University Press, 1992.
- G. R. Desiraju, *Crystal Engineering: Designing of Organic Solids*, Elsevier, New York, 1989.
- D. Braga, F. Grepioni and A. G. Orpen, *Crystal Engineering: from Molecules and Crystals to Materials*, Kluwer Academic Publishers, Dordrecht, 1999.
- U. Schubert and N. Husing, *Synthesis of Inorganic Material*, 2nd Edn., Wiley-VCH Verlag GmbH & Co., Weinheim, 2005
- J. N. Lalena and D. A. Cleary, *Principles of Inorganic Materials Design*, Wiley-Interscience, New Jersey, 2005.
- X. -D. Xiang and I. Takenchi (Eds.), *Combinatorial Synthesis*, Marcel Dekker, New York, 2003.
- E. I. Stiefel (Ed), *Dithiolene Chemistry: Synthesis, properties, and Applications*, John Wiley & Sons, New Jersey, 2004.
- P. Gomez-Romero and C. Sanchez (Eds.), *Functional Hybrid Materials*, Wiley-VCH, Weinheim, 2004.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1993.
- 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 Edb, Cambridge University Press, Cambridge, 1964.
- W. E. Addison, *Structural Principles in Inorganic Compounds*, John Wiley, New York, 1961.

CS 403: Nuclear-Analytical Special

Group A

1. Trace and ultra-trace analysis — an instrumental approach: (14 lectures)

Introduction to various instrumental methods for trace and ultra-trace analysis — atomic absorption, flame photometry, atomic emission, atomic fluorescence — theory,

instrumentation and application, Raman spectroscopy — Raman effect, applications, spectra of typical molecules, photochemistry — laws, quantum yield — problems, instrumentation, examples of photochemical reactions, actinometer, molecular luminescence spectrometry — theory, instrumentation, application, effect of temperature and solvent effects in fluorescence

2. Kinetic method of analysis: (13 lectures)

Introduction, transition state theory, dielectric effect and ion-ion interaction, study of fast reaction, stopped flow, relaxation method, reaction involving structural changes and enzymatic processes; template reaction; self-exchange reaction, electron tunneling hypothesis, Marcus theory: inner-sphere and outer-sphere reaction, indicator reactions, application of kinetic methods in trace analysis.

Group B

3. Some recent analytical techniques: (09 lectures)

Hyphenated techniques — state of art, GC-MS, LC-MS, GC-FTIR, GC-MS-FTIR, GC-AED, LC-FTIR, LC-NMR

4. Applied analysis: (09 lectures)

Sampling, modern methods of sample digestion, typical analysis of ores, minerals, alloys, glass and ceramic materials, fuel, food, food additives, drug, pesticides in fruit juice and water

5. Basic electronics (09 lectures)

Characteristics and use of diodes, capacitors, inductors, transformers, FET, MOSFET, rectifier, power supply, clipper, oscillator and timer circuits, linear small signal amplifiers and their characteristics, integrated circuits, operational amplifier and its applications including applications in analytical and nuclear instruments, logic gates and elementary digital circuits

List of Recommended Books/Journals

- I. M. Kolthoff, P. J. Elving and E. B. Sandell, *Treatise on Analytical Chemistry*, Pt-I, II, III, The Interscience Encyclopedia, Inc., New York, 1959.
 A. I. Vogel, *A Test Book of Quantitative Inorganic Analysis*, 3rd Edn., Longmans, 1961.
 D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill, New York, 2000.
 D. A. Skoog, *Principle of Instrumental Analysis*, 3rd Edn, Saunders College Publishing, New York, 1985.
 D. A. Skoog and J. J. Leory, *Principles of Instrumental Analysis*, Saunders, Philadelphia, 1994.

- G. D. Christian, *Analytical Chemistry*, 5th Edn. John Wiley, New York, 1994.
- R. J. H. Clark and R. E. Hester, *Advances in Infrared and Raman Spectroscopy*, John Wiley, 1985.
- D. Rendell and D. Mowthrope, *Fluorescence and Phosphorescence Spectroscopy*, John Wiley, 1987.
- E. Metcalfe and F. E. Prichard, *Atomic Absorption and Emission Spectroscopy*, John Wiley, 1987.
- P. W. J. M. Boumans, *Inductively Coupled Plasma Emission Spectroscopy*, John Wiley, 1987.
- K. E. Jarvis, A. L. Gray and R. S. Houlk, *Hand Book of Inductively Coupled Plasma Emission Spectroscopy*, Blackie, Classgow and London, 1992.
- D. J. Peters, J. H. Hayes and G.M. Hieftje, *Chemical Separation and Measurements*, Saunders, Philadelphia, 1974.
- A. Welz, *Atomic Absorption Spectrometry*, Verlag, Weinheim, 1985.
- W. Salvin, *Graphite Furnace AAS: A Source Book*, Perkin-Elmer, Norwalk, 1984.
- G. W. Ewing, *Instrumental Methods of Chemical Analysis*, 4th Edn., McGraw Hill, 1978.
- E. Y. Wehry, *Modern Fluorescence Spectroscopy*, Plenum Publishing Company, 1981
- K. Nakamoto, *Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds*, Wiley, 1986.
- H. M. Kingston and L. B. Jassie (Ed), *Introduction to Microwave Sample Preparation: Theory and Practice*, American Chemical Society, Washington DC, 1988.
- S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, New Age International Ltd. Publishers, New Delhi, 1998.
- D. A. Skoog, d. M. West and F. J. Holler, *Fundamentals of Analytical Chemistry*, 7th Edn., Saunders, Philadelphia, 1996.
- R. Kellner, J. M. Mermet, M. Otto and H. M. Widmer (Ed), *Analytical Chemistry*, Wiley-VCH, Weinheim, 1998.
- J. D. Ingel, Jr. and S. R. Crouch, *Spectroscopic Analysis*, Prentice Hall, New Jersey, 1988.

CS 403: Organic Special

Group A

- Orbital symmetry and pericyclic reactions: (18 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 transistion state concept (qualitative); topology of cyclo-additions, periselectivity, regioselectivity, Lewis acid catalysis; higher order cyclo-additions, dipolar additions, electrocyclic reactions, sigmatropic reactions, chelotropic reaction, ene reactions, selection rules
- Asymmetric synthesis: (09 lectures)
The chiral pool; chiral auxiliaries, reagents and catalysts; Diels-Alder reaction, Heck reaction; alkylation of chiral enolates; didydroxylation.

Group B

3. Steroids (05 lectures)
 Reactions and synthesis of steroids, sources of steroid hormones, diosgenin, hecogenin
4. Nucleic acids: (17 lectures)
 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
5. Heterocyclic Chemistry: (05 lectures)
 Structure, synthesis and reactivity of 5,6-membered rings containing two heteroatoms, pyrimidines and purines

Tentative List of Recommended Books/Journals

- T.L. Gilchrist and R.C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn., Cambridge University Press, 1979.
- R.B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.
- R. Streitwieser, *Molecular Orbital Theory of Organic Chemists*, John Wiley, 1961.
- E.R. Lehr and A.P. Merchand, *Orbital Symmetry and Cyclo-addition*, Academic Press, 1972.
- G. B. Gills and M. R. Willis, *Pericyclic Reactions*, Chapman and Hall, 1974.
- T.H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn., Harper and Row, 1998.
- I. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, John Wiley, 1980.
- F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4th Edn., Plenum Press, 2001.
- R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley, 1994.
- R.E. Ireland, *Organic Synthesis*, Prentice-Hall, 1969.
- R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3rd Edn., ELBS, 2003..
- W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn., Low Price Edition, Cambridge University Press, 1996.
- A. H. Depuy and O.H. Chapman, *Molecular Reaction and Organic Photochemistry*, Prentice-Hall, 1975.
- J.S. Bindra and R. Bindra, *Prostaglandin Synthesis*, Academic Press, 1983.
- L.F. Fieser and M. Fieser, *Steroids*, Reinhold, 1967.

- L.J. Goad and T. Akisha, *Analysis of Sterols*, Blackie Academic and Professional, 1997.
 G. Thomas, *Medicinal Chemistry – An Introduction*, John Wiley, 2001.
 R. L. Pecsok, L. D. Shields, T. Cairns and Ian G. McWilliam, *Modern Methods of Chemical Analysis*, 2nd Edn., 1996.
 A. Mazur and B. Harrow, *Text Book of Biochemistry*, 10th Edn., W.B. Saunders Co., 1971.
 P.W. Kuchel and G.B. Ralston, *Theory and Problems in Biochemistry*, International Edition, McGraw-Hill, 1988.
 D.L. Nelson and M.M. Cox, *Lehninger: Principle of Biochemistry*, 4th Edn., W.H. Freeman Co., 2005.
 T. M. Devlin, *Text Book of Biochemistry*, 2nd Edn., John Wiley, 1986.
 J.M. Berg, J.L. Tymoczko & L. Stryer, *Biochemistry*, 5th Edn., W.H. Freeman Co., 2002.
 R. M. Acheson, *Introduction of Chemistry of Heterocyclic Compounds*, 2nd Edn., Interscience Publisher, 1967.

CS 403: Physical Special

Group A

1. Principles of quantum mechanics: (27 lectures)

Analysis of the postulates — pictures and representations; Ehrenfest's theorem; uncertainty principle; properties of sets of functions, Schmidt orthonormalisation; Fourier transformation, delta function with examples, free particle normalization; matrix formulation, tunneling, bound states, the Virial theorem

Group B

2. Approximate methods in quantum mechanics: (12 lectures)

Time dependent perturbation theory, semiclassical treatment of radiation-matter interaction, transition probability and rates, Einstein's A and B coefficients, selection rules; principles of linear and non-linear variation methods, stationary perturbation theory for non-degenerate and degenerate states — applications to rotator, Stark effect, the He-atom

3. Quantum chemistry: (15 lectures)

Antisymmetry of many electron wave function, spin and spatial orbitals, Slater determinant; closed-shell and open-shell electron configurations; multi-electron pure-spin state wave functions — examples with 2- and 3-electron systems, formulation of a multi-electron closed-shell electron configuration energy, introduction of core, Coulomb and exchange integrals with their properties — example of He atom, independent particle model, multi-electron atomic Hartree Hamiltonian and related SCF equations solution,

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

Tentative List of Recommended Books/Journals

- 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.
 S P. C. W. Davies, *Quantum Mechanics*, ELBS, 1985.
 J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, 1961.
 D. Bohm, *Quantum Theory*, Asia Pub. House, 1960.
 R. McWeeny, *Methods of Molecular Quantum Mechanics*, Academic Press, London, 1989.
 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.

Practical

CSP 404: Inorganic Special

1. Preparation of inorganic and coordination compounds and their characterization
 - a. Bi-, tri-, and polydentate ligands
 - b. Complexation and purification
 - c. Growing of single crystals
 - d. Elemental analyses (C, H, N and AAS)
 - e. Spectral, thermal, electrochemical and magnetic studies
2. Kinetic and mechanistic studies of some selected reactions (substitution and redox)

CSP 404: Nuclear-Analytical Special

1. Experiments with GM detector
2. Use of γ -ray spectrophotometer
3. Some radioanalytical experiments

CSP 404: Organic Special

1. Preparation of organic compounds involving multiple step reactions
2. Characterization of organic compounds using spectrophotometric methods

CSP 404: Physical Special

1. Instrumental methods of studying hydrolysis, solubility and kinetics; elementary computer-based numerical methods
2. Methods of determination of molecular weights of solids and liquids

CCA 405: Computer Application in Chemistry**A. Theoretical (30 lectures)****1. Introduction to computers:**

Scope for computers, present-day position, computer overview and organization; hardware: CPU, memory – volatile and non-volatile, I/O devices and controllers; software: concept of stored programmes, information storage and retrieval, control instructions and data, idea of operating system, driver and controller programmes, utility packages, user programmes and code

2. Number system:

Decimal, binary, octal and hexadecimal representations, negative numbers and floating point numbers, character sets (ASCII, EBCDIC), fixed and floating point arithmetic

3. Introduction to DOS and WINDOWS

Concept of file, record, data, bit, byte, block; track, sector on storage media; use of file editors — EDIT, NORTON, word Processors etc.

4. Introduction to DOS and WINDOWS:

Data types, arithmetic operations and expressions, relational expressions, library functions, I/O and format statements, control statements, nesting of loops, block IF, subroutines and function subprograms, subscribed variables, dimension and common, parameter passing between programme modules, file handling (OPEN, CLOSE, INQUIRE, REWIND, BACKSPACE, ENDFILE)

5. Numerical techniques and chemical applications:

Algorithms, logical analysis of problems, flow-chart, programmes, data fitting by least square, interpolation techniques, iterative methods, solution of simultaneous equations

B. Practical (20 lab hours)

On-hand practical training with computers on selected chemical problems

Tentative List of Recommended Books/Journals

S. Lipschutz, A. Poe, Programming with FORTAN (Schaum Series), Mc-Graw-Hill International Edition, Singapore, 1982.

V. Rajaraman, Computer programming in FORTAN IV, PHI, New Delhi, 1982.

B. W. Kernighan, D. M. Ritchie, The C programming Language, PHI, Eastern Economy Edition, New Delhi, 1996.

V. Rajaraman, Computer programming in C, PHI, New Delhi, 1996.

R. S. Salaria, Numerical Methods, B. P. B. Publications, New Delhi, 1996.

S. D. Conte and C. de Boor, Elementary Numerical Analysis, McGraw-Hill International, New Delhi, 1986.

E. G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer (India) Pvt. Ltd., 2007.

CTP 406: Term paper

Topic selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted; seminar lecture on this topic to be delivered in presence of all the teachers.