SYLLABUS (CBCS)

For

M.Sc. Course in Chemistry

To be effective from the session 2017-19

BANKURA UNIVERSITY

BANKURA -722155

WEST BENGAL, INDIA

Credits & Evaluation

Duration of PG Course of Studies in Chemistry will be of two years with four Semesters, viz., Semester I, Semester II, Semester III and Semester IV - each of six months' duration coupled with four examinations *viz*. Semester I, Semester II, Semester III and Semester IV in chemistry at the end of each Semester. Syllabus is hereby framed according to certain schemes and structures highlighted below Schemes:

1. 300 marks in each Semester with a grand total of 1200 marks and 96 credits.
2. 24 credits in each Semester with a total of 96 credits; each theoretical/practical paper of 4 credits.
3. 20% marks allotted for internal assessment in each theoretical paper which will be assessed by written test conducted by the department.
4. 20% marks allotted for internal assessment in each practical paper which will be assessed either by written test or viva-voce conducted by the department.
5. Three theoretical papers (common to all students) in each of Semester I, Semester II and Semester III.
6. Two practical papers (common to all students) in each of Semester I, Semester II and Semester III.
7. Three major electives *viz.* Inorganic, Organic and Physical in Semester IV; number of students in each

   Major paper to be decided by the department;
8. In Semester III, one Extra Departmental elective paper to be learnt by the students of the other sister departments and the students of this department be learnt from other sister departments.
9. In Semester IV, one paper on term paper/project work (subject matter of each major paper of Semester IV)
10. Duration of examination: each theoretical paper of 2 hours, each practical paper, 6 hours
11. For each practical paper: experiments, 40; viva-voce (by external examiner), 10
12. For term paper/project work: Preparation 25, presentation of seminar in presence of external expert; 15, and thereafter interaction,10

Course Structure

	Paper Code	Core Subject	Marks				Credit
			IA	ESE		TOTAL	
				TH	PR		
SEMESTER I	**Theoretical Papers**						
	CHEM 101C	Inorganic Chemistry	10	40	-	50	4
	CHEM 102C	Organic Chemistry	10	40	-	50	4
	CHEM 103C	Physical Chemistry	10	40	-	50	4
	Practical Papers						
	CHEM 104C(PR)	Inorganic Chemistry Practical	10	-	40	50	4
	CHEM 105C(PR)	Organic Chemistry Practical	10	-	40	50	4
	106CF	*Compulsory Foundation (Communicative English & Personality Development)				50	-
	CHEM 107I.A.	**Internal Assignment				50	4
		Total				**300**	**24**

	Paper Code	Core Subject	Marks				Credit
			IA	ESE		TOTAL	
				TH	PR		
SEMESTER II	**Theoretical Papers**						
	CHEM 201C	Inorganic Chemistry	10	40	-	50	4
	CHEM 202C	Organic Chemistry	10	40	-	50	4
	CHEM 203C	Physical Chemistry	10	40	-	50	4
	Practical Papers						
	CHEM 204C(PR)	Inorganic Chemistry Practical	10	-	40	50	4
	CHEM 205C(PR)	Physical Chemistry Practical	10	-	40	50	4
	206EF	*Elective Foundation (Value Education and Human Rights)				50	-
	CHEM 207I.A.	**Internal Assignment				50	4
		Total				**300**	**24**

	Paper Code	Core Subject	Marks				Credit
			IA	ESE		TOTAL	
				TH	PR		
SEMESTER III	**Theoretical Papers**						
	CHEM 301C	Inorganic Chemistry	10	40	-	50	4
	CHEM 302C	Organic Chemistry	10	40	-	50	4
	CHEM 303C	Physical Chemistry	10	40	-	50	4
	Practical Paper						
	CHEM 304C(PR)	Organic Chemistry Practical	10	-	40	50	4
	#Elective Course						
	CHEM 305 EID	Advanced General Chemistry	10	40	-	50	4
	Practical Paper						
	CHEM 306C(PR)	Physical Chemistry Practical	10	-	40	50	4
		Total				**300**	**24**

	Paper	Core Subject	Marks				Credit
			IA	ESE		TOTAL	
				TH	PR		
SEMESTER IV	**Theoretical Papers**						
	CHEM 401E (IS/OS/PS)	Special Theory	10	40	-	50	4
	CHEM 402E (IS/OS/PS)	Special Theory	10	40	-	50	4
	CHEM 403E (IS/OS/PS)	Special Theory	10	40	-	50	4
	Practical Papers						
	CHEM 404C(PR)	Computer Application in Chemistry	10	-	40	50	4
	CHEM 405E(PR) (IS/OS/PS)	Special Practical	10	-	40	50	4
	##Term Paper/Project						
	CHEM 406I.A. (IS/OS/PS)	Term Paper/Project	Preparation-25; Presentation-15; Viva-voce-10				4
		Total				**300**	**24**
		Grand Total	**1200**				**96**

(IS): Inorganic Special; (OS): Organic Special; (PS): Physical Special

C = Core Course; E = Elective; CF = Compulsory Foundation Course; EF= Elective Foundation; EID = Elective Interdisciplinary; TH = Theory; PR = Practical; IA = Internal Assessment; I.A. = Internal Assignment; ESE = End Semester Examination:

***** The foundation courses are to be conducted by the University. The course shall have internal assessment only and so, credit earned for these courses, shall not be considered while preparing the final result. However, the candidates are required to obtain Satisfactory or Not Satisfactory to become eligible for the final semester examination/award of the PG Degree.

**Internal Assignment: Assignment (15 marks), Seminar (30 marks), Tutorial (5 marks)

Courses are mandatory choice based and students (other than the Department of Chemistry) of any Department of PG level may opt for the course. Classes will be held on Monday, Wednesday, Thursday and Friday from 1.00 pm to 2.00 pm)

For term paper/project: Preparation + Presentation + Viva-voce = 25 + 15 + 10 = 50.

Semester I (Total Marks-300, Credit-24)

Theoretical Papers

CHEM 101C: Inorganic Chemistry **Marks: 50, Credit: 4**

1. Chemistry of Coordination Compounds

Classification of ligands, stability, reactivity, bond types, geometry and coordination compounds. Design of specialized ligand. chelator/congregator. Non-transition and transition metal ion homoleptic/heteroleptic and homonuclear/heteronuclear complexes of different dimensions with varied mono- and polydentate blockers containing carbon, nitrogen, phosphorus, chalcogen, halogen donors with/without mono-/polydentate bridges and counter ions. Polyhedra for coordination and cluster compounds. Isoelectric and Isolobal relationship.

Electronic spectra of transition metal complexes: Microstates, Russell-sander's terms, determination of ground and excited state terms of d^n ions; Orgel diagrams (qualitative approach), selection rules for spectral transitions, *d-d* spectra of d^n ions and crystal field parameters, nephelauxetic series.

2. Organometallic Chemistry

Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study. Metal-alkyl, -allyl, -aryl, -carbene (Fischer and Schrock type), -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity. Polyalkyls and polyhidrides complexes. Organoboron and Organoaluminium compounds.

3. Electro- and Thermo-analytical Techniques

Introduction to electrochemical methods, electrochemical cells, current – voltage relationship during electrolysis. Principles and applications of Voltammetry, cyclic voltammetry, coulometry, electrogravimetry.

Thermal analysis: definition and uses. Thermogravimetry: application, TGA curve analysis. Differential Thermogravimetry: DTA, DSC.

4. Metal-Ligand Equilibria in Solution

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed

ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic and template effect.

5. Advanced Bioinorganic Chemistry

Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer. Redox enzymes: Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase; molybdo enzymes: xanthene oxidase, nitrate reductase, sulfite oxidase including some model study. Vitamins and coenzymes: Vitamin B_6 and vitamin B_{12} coenzymes. Carcinogenicity of chromium. Selenium in biology.

Reference Books

- J. D. Lee, *Concise Inorganic Chemistry*, ELBS, 1991.
- B. E. Douglas and D. H. McDaniel, *Concepts & Models of Inorganic Chemistry*, Oxford, 1970.
- R. H. Crabtree, *The Organomettalic Chemistry of the Transition Metals*, 4th Edn, Wiley, New York, 2005.
- P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn, Chapman and Hall, London, 1988.
- G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, International 2nd Edn, Oxford University Press, Oxford, 2010.
- A. Yamamoto, *Organotransition Metal Chemistry*, Wiley, New York, 1986.
- M. C. Day and J. Selbin, *Theoretical Inorganic Chemistry*, ACS Publications, 1962.
- P. Atkin, Shriver & Atkins *Inorganic Chemistry*, 5th Edn. Oxford University Press, 2010.
- F. A. Cotton, G. Wilkinson and P. L. Gaus, *Basic Inorganic Chemistry*, 3rd Edn, Wiley India, 1995.
- J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry, Principles of Structure and Reactivity*, 4th Edn, Harper Collins 1993, Pearson, 2006.
- F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, New York, 1967.
- D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.
- R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
- S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, CA, 1993.
- A. K. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, 2nd Edn, U. N. Dhur and Sons, Kolkata, 2002.
- A. K. Das, *Bioinorganic Chemistry*, Books & Allied (P) Ltd. Kolkata 2007.
- E. Ochiai, *Bioinorganic Chemistry: A Survey*, Academic Press, Elsevier, 2009.

CHEM 102C: Organic Chemistry **Marks: 50, Credit: 4**

1. Bonding in Organic Molecules

Qualitative M.O. treatment to acyclic and cyclic conjugated systems. Huckel treatment-applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene and benzene. Concept of aromaticity in benzenoid, and non benzenoid systems. Alternant and non-alternant hydrocarbons. Aromaticity in annulenes, hetero-annulenes and fullerenes (C_{60}). Examples of anti-aromaticity and homo aromaticity. Graphical method- Frost diagram. Linear free energy relations: Hammett equation; equilibria and rates in organic reactions; separation of polar, steric and resonance effects: Taft equation, Grunwald -Winstein equation.

2. Stereochemistry and Conformational Analysis-I

Molecular symmetry, chirality and point group; stereoisomerism: definitions, classifications; configuration and conformation; relative and absolute configuration; determination of relative configuration: Prelog's rule, Cram's rule, and Sharpless rule; conformations of acyclic and cyclic system (3 to 8 membered rings), fused (5/5 and 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)

3. NMR Spectroscopy

Principles, instrumentation and different techniques (CW and FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J); Jablonski diagram, spin-decoupling. First order and second order spectra, spin system notations. Introduction to ^{13}C: proton decoupled ^{13}C spectra, NOE, cross polarization, peak integration, off resonance ^{13}C.

4. Mass Spectroscopy

Mass Spectroscopy Principles, instrumentation and applications of mass spectrometry-methods of generation of ions in EI, CI, FD and FAB, MALDI-TOF. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotope, ion-molecule interaction and analysis of fragmentation patterns. Calculation of MF from mass.

Applications of Mass, UV-VIS, IR and NMR spectroscopy to structural and mechanistic problems.

Reference Books

- E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2006.
- S. Shaik, and P. C. Hiberty, *Valence Bond Theory, Its History, Fundamentals, and Applications: A Primer, In: Reviews in Computational Chemistry*, Volume 20 (Eds. K. B. Lipkowitz, R. Larter and T. R. Cundari), John Wiley & Sons, Inc., Hoboken, NJ, USA, 2004.
- F. A. Carroll, *Perspectives on Structure and Mechanism in Organic Chemistry*, 2nd Edn, Wiley-VCH, 2011.
- E. L. Eliel, S. H. Wilson and L. N. Mander, *Stereochemistry of Organic Compounds*, John Wiley & Sons, Inc., 2003.
- E. L. Eliel, *Stereochemistry of Carbon Compounds*, Tata McGraw-Hill Edition, New Delhi, 1988.
- D. Nasipuri, *Stereochemistry of Organic Compounds (Principles and Applications),* 2nd Edn, Wiley Eastern Limited, New Delhi, 1994.
- E. L. Eliel, N. L. Allinger, S. J. Angyal and G.A Morrison, *Conformational Analysis*, John Wiley & Sons, Inc., 1967.
- J. Eames and J. Peach, *Stereochemistry at a Glance*, Blackwell Science, 2003.
- K. Mislow and W. A. Benjamin, *Introduction to Stereochemistry*, New York, 1965.
- B. Testa, *Principles of Organic Stereochemistry*, Marcel Dekker, New York, 1979.
- E. Juaristi, *Stereochemistry and Conformational Analysis*, John Wiley & Sons, Inc., 1991.
- M. Nogradi, *Stereochemistry: Concepts and Applications*, Pergamon Press, New York, 1981
- H. -J. Zhu, *Organic Stereochemistry: Experimental and Computational Methods*, Wiley-VCH, 2015.
- M. B. Smith and J. March, *March's Advanced Organic Chemistry (Reactions, Mechanisms, and Structure)*, 5th Edn, John Wiley & Sons, Inc., 2001.
- L. N. Ferguson, *The Modern Structural Theory of Organic Chemistry*, Prentice-Hall of India Pvt. Ltd., New Delhi, 1963.
- R. H. Grubbs and D. J. O'leary (Eds), *Handbook of Metathesis* – Vols. 1 and 2, Wiley-VCH, 2015.
- D. L. Pavia, G. M. Lampman and G. S. Kriz, *Introduction to Spectroscopy*, 3rdEdn, Harcourt, Inc., 2001.
- R. M. Silverstein, G. C. Bassler and T. C. Morrill, *Spectroscopic Identification of Organic Compounds*, 5th Edn, John Wiley & Sons, Inc., 1991.
- D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5th Edn., Tata McGraw-Hill Edition, New Delhi, 2004.
- W. Kemp, *Organic Spectroscopy*, 3rd Edn, Macmillan Press Ltd., 1991.

- G. Siuzdak, *Mass Spectrometry for Biotechnology*, Academic Press, 2005.
- H. Budzikiewicz, C. Djerassi and D. H. Williams, *Interpretation of Mass Spectra of Organic Compounds*, Holden-Day Inc., 1965.
- J. S. Splitter and F. Tureček,*Applications of Mass Spectrometry to Organic Stereochemistry*, Wiley-VCH, 1994.
- Atta-ur-Rahman and Md. Iqbal Choudhary, *Solving Problems with NMR Spectroscopy*, Academic Press, Inc., 1996.
- N. S. Bhacca and D. H. Williams, *Applications of NMR Spectroscopy in Organic Chemistry*, Holden-Day, Inc., 1964.
- L. M. Jackman and S. Sternhell, *Applications of Nuclear Magnetic Resonance Spectroscopy In Organic* Chemistry, 2nd Edn., Pergamon Press, Oxford. 2nd Edn, 1969.
- R. G. Linington, P. G. Williams and J. B. MacMillan, *Problems in Organic Structure Determination: A practical Approach to NMR Spectroscopy*, CRC Press, Taylor & Francis Group, 2016.

CHEM 103C: Physical Chemistry **Marks: 50, Credit: 4**

1. The Foundations of Quantum Mechanics

Historical background of quantum mechanics: Wave-particle duality, Uncertainty principle, Postulates of Quantum Mechanics; Schrodinger wave equation and its solution; Wavefunction and its probabilistic interpretation, well behaved functions, orthonormality: Orthogonality and normalization of wavefunctions; operator algebra, Observable, linear and nonlinear operators, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, eigen functions of commuting operators; Expectation value postulate; Postulate of Time-Dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation.

2. Free particle and Particle-in-Box

Particle in a one-dimensional box with infinite potential walls, important features of the problem; Free particle in one -dimension; Particle in a one-dimensional box with finite potential walls (or particle in a rectangular well) – tunneling; Particle in a three dimensional box, separation of variables, degeneracy, Discussion on Bohr's correspondence principle.

3. Group Theory-I

Introduction to symmetry. Symmetry elements and Symmetry operations. Definition of a Group. Point symmetry groups. Group multiplication tables. Theorems of groups. Conjugate elements and class.

Symmetry Operators and their Matrix Representation. Function space. Reducible and irreducible representations. Equivalent representations. Characters of representations.

4. Electrochemistry

Introduction, ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Solvation and 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.

5. Chemical kinetics

Theories of reaction rates: applications to uni-, bi- and termolecular reactions, thermodynamic formulation of reaction rate, reactions in solution; cage effect, 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; flow process and relaxation techniques.

Reference Books

- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- R. Taylor, *The Chemistry of Fullerenes, Advanced Series in Fullerenes*, Vol 4, World Scientific, Singapore, 1995.
- D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.
- N. R. Rao, A. Müller, A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, Vols 1 and 2, Wiley-VCH, Weinheim, 2004.
- P. Bréchignac, Houdy, M. Lahmani, *Nanomaterials and Nanochemistry*, Springer, London, 2006.
- N. Levine, *Physical Chemistry*, Tata McGraw-Hill, New Delhi, 1978.
- 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.
- 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, New York, 1995.

- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.
- K. J. Laidler, *Reaction Kinetics*, Vols I and II, Pergamon Press, London, 1970.
- L. P. Hammett, *Physical Organic Chemistry*, McGraw-Hill Book Company, New Delhi, 1970.
- J. Albery, *Electrode Kinetics*, Oxford Chemistry Series, Clarendron Press, Oxford, 1975.
- K. J. Laidler, *Chemical Kinetics*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.
- M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.

Practical Paper

CHEM 104C(PR): Inorganic Chemistry Practical Marks: 50, Credit: 4

1. Analysis of Complex Materials

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional (volumetric, complexometric, gravimetric) and or instrumental methods as applicable.

Model Samples - Ores, Minerals, Concentrates: Dolomite ($CaCO_3$, $MgCO_3$, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys: Brass (Cu, Zn); Soldier/Type metal (Pb, Sb, Sn); Bronze (Cu, Zn, Sn), Aluminium bronze (Cu, Al, Fe, Mn), Steel (Cr, Mn, Ni, P). 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.

CHEM 105C(PR): Organic Chemistry Practical Marks: 50, Credit: 4

1. Qualitative Organic Analysis

Identification of single liquid organic compound by physical and chemical tests and preparation of at least one suitable solid derivative after consulting literature. Functional groups include: amino- (1°, 2°, 3°), anilido-, nitro-, cyano-, alkcoholic –OH, phenolic –OH, enols, carbonyl

(aldehydo-, keto-) carboxylic acids, esters, unsaturation and hydrocarbons. (at least six experiments to be performed in class).

2. Short Organic Synthesis

A. Oxidation of benzylic carbon by prior protection of $-NH_2$ group in the nucleus followed by deprotection: 4-Aminotoluene 4-Aminobenzoic acid.

B. Preparation of imide followed by Hofmann degradation: Phthalic anhydride Anthranilic acid.

C. Reductive removal of aromatic amino group by prior diazotization followed by Sandmeyer reaction.

D. Oxidation of α-hydroxyketone to diketone followed by rearrangement: Benzoin Benzilic acid.

E. 1,4-Dihydropyridine ring generation: Ethyl acetoacetate 2,6-Dimethyl-3,5-dicarbethoxy-1,4-dihydropyridine.

F. Partial reduction of aromatic dinitro compound: m-Dinitrobenzene *m*-Nitroaniline.

G. Benzoylation of amino group in presence of carboxylic acid group: Glycine Hippuric acid.

H. Reduction of a hydroxycarboxylic acid with HI and red P: Benzilic acid. Diphenylacetic acid.

At least four experiments to be performed in class on a rotation basis.

Semester II (Total Marks-300, Credit-24)

Theoretical Papers

CHEM 201C: Inorganic Chemistry Marks: 50, Credit: 4

1. Inner Transition Elements: Spectral and Magnetic Properties, Redox Chemistry, Analytical Applications

Comparison of characteristics of Inner Transition and Transition metals. Source, extraction and application. Stable oxidation states. Coordination numbers and stereochemistry. Mono- and polynuclear compounds of lanthanoid and actinoid ions stressing on choice of different multidentate chelators and congregators with special emphasis on electric, magnetic, conducting, superconducting and fluorophoric behaviours. Magnetic properties and absorption spectra of Lanthanoids and Actinoids. Coordination complexes of oxygen donor ligands. Organometallic compounds of Ln and An. Lower oxidation state compounds. General chemistry of Actinoids. Reactivity of organometallic compounds of *f* -block elements.

2. Structure and Properties of Solids

Fundamentals, ionic, covalent, hydrogen bonded and molecular solids; perovskite, ilmenite and rutile; spinel and inverse spinel, diamond cubic, 3D network, pyroxene, amphibole, talc, mica, crystal defects, non-stoichiometric compounds; electronic properties of solids, F-centre, conductors, insulators, semiconductors, superconductors; ferroelectricity, antiferroelectricity, pyroelectricity, piezoelectricity, liquid crystals, cooperative magnetism. History of Nanoscience, Nano-world definitions, Properties of Nanomaterials, Typical synthetic strategies for nanomaterials, Modern characterization methods and Applications of nanomaterials in different areas.

3. Inorganic Chains, Rings, Cages and Clusters

Phosphazenes. Homo- and Heterocyclic inorganic ring systems. Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds- Lipscomb's topological models, Wade's rules, polyhedral skeletal electron pair theory (PSEPT), carboranes and metallacarboranes. Metal Clusters, Giant Clusters and synthesis methedology. Metal-metal bonding, single and multiple bonded compounds. Low and high nuclearity clusters. Electron counting and structure of clusters, Wade-Mingos-Lauher rule. Structure and isolobal analogies. Polyatomic Zintl cations and anions. Chevrel Phases. infinite metal chains, multidecker molecules, cluster-surface analogy.

4. Clays and Zeolites

Characterization of Clays, zeolitic structures, surface area, surface activity, pore size, application of clays and zeolites, MOFs with zeolitic structure. Reticular syntheses.

5. Silicates and Aluminosilicates

Classification, structure, properties and application of naturally occurring silicates and aluminosilicates, silicates: single/double chain.

Reference Books

- J. D. Lee, *Concise Inorganic Chemistry*, ELBS, 1991.
- B. E. Douglas, and D. H. McDaniel, *Concepts & Models of Inorganic Chemistry*, Oxford, 1970.
- M. C. Day, and J. Selbin, *Theoretical Inorganic Chemistry*, ACS Publications, 1962.
- N. N. Greenwood, and A. Earnshaw, *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
- P. Atkin, Shriver and Atkins *Inorganic Chemistry*, 5th Ed. Oxford University Press (2010).
- F. A. Cotton, G. Wilkinson, and P. L. Gaus, Basic Inorganic Chemistry, 3rd Edn, Wiley India.
- J. E.. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edn, Harper Collins 1993, Pearson, 2006.
- B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
- G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edn, Pearson, New Delhi, 2009.
- D. M. P. Mingos and D. J. Wales, *Introduction to Cluster Chemistry*, Prentice Hall, New York, 1990.
- D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds), *The Chemistry of Metal Cluster Complexes*, VCH, New York, 1990.
- C. E. Housecroft, *Cluster Molecules of the p-Block Elements*, Oxford University Press, Cambridge, 1994.
- K. J. Klabunde, *Free Atoms, Clusters and Nanoscale Particles*, Academic Press, New York, 1994.
- W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds*, Dover Publications, New York, 1989.
- D. M. Adams, *Inorganic Solids*, Wiley, New York, 1992.

CHEM 202C: Organic Chemistry **Marks: 50, Credit: 4**

1. Heterocyclic Chemistry-I

Systematic nomenclature (Hantzch-Widman system) for monocycle and fused heterocycles. General approach to heterocyclic synthesis-cyclisation and cycloaddition routes. Heterocycles in organic synthesis-masked functionalities, umpolung, Stork annulations reaction. Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

2. Organic Name Reaction and Reagents

Baeyer-Villiger oxidation; Barton reaction; Beckmann rearrangement; Birch reduction; Claisen rearrangement; Favorskii reaction; Fries rearrangement; Heck reaction; Mannich reaction; McMurry reaction; Michael addition; Perkin reaction; Sharpless asymmetric epoxidation; Stile coupling; Strecker reaction; Suzuki coupling; Wittig reaction; Yamaguchi esterification. Hydride transfer reagent: Boranes, trialkyl borohydrides, Diimide, Baker's yeast, trialkyl tin hydride; DIBAL, $Na(CN)BH_3$, Woodward and Prevost hydroxylation, Sharpless epoxidation, PCC, PDC, Mn(IV) oxide, RuO_4 (TPAP), Moffat oxidation, Swern oxidation, Dess-Martin Periodinane; Shapiro reaction, Peterson reaction, OsO_4, SeO_2.

3. Pericyclic Reactions-I

Classification of pericyclic reactions. Theory of pericyclic reactions (i) Frontier Molecular Orbital (FMO) approach, (ii) Concept of aromaticity of transition states (Huckel/Mobius systems). Thermal and photopericyclic reactions, The Woodward-Hoffmann selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, carbene addition, cheleotropic reactions. Rationalization based on Frontier M.O. approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Sommelet-Hauser, Cope, aza-Cope and Claisen rearrangements, Ene Reaction. Wittig rearrangement, suitable examples of [(2Π +2 Π), (4Π +2 Π), (4Π + 4Π), (2Π +2Π+2Π)] and metal catalysed cycloaddition reactions.

4. Asymmetric Synthesis

The chiral pool: synthesis and application; asymmetric Diels-Alder reaction, Heck reaction and Aza-Baylis–Hillman reaction. Enantioselective organocatalysis, Biocatalysis.

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Reference Books

- T. L. Gilchrist and R. C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn, Cambridge University Press, 1979.
- N. J. Turro, *Modern Molecular Photochemistry*, The Benjamin Cummings Publishing Co., Inc., 1978.
- S. Sankararaman, *Pericyclic Reactions – A Textbook*, Wiley-VCH Verlag, 2005.
- R. E. Gawley and J. Aube, *Principles of Asymmetric Synthesis*, Elsevier, 1996.
- M. Gruttadauria and F. Giacalone, *Catalytic Methods in Asymmetric Synthesis: Advanced Materials, Techniques, and Applications*, John Wiley & Sons, 2011.
- I. Ojima, *Catalytic Asymmetric Synthesis*, John Wiley & Sons, 2013.
- G. -Q. Lin, Y. -M. Li and A. C. Chan, *Principles and Applications of Asymmetric Synthesis*, John Wiley & Sons, 2003.
- M. P. Koskinen, *Asymmetric Synthesis of Natural Products*, John Wiley & Sons, 2012.
- J. A. Joule and K. Mills, *Heterocyclic Chemistry*, Blackwell Science Publication, 2000.
- R. K. Bansal, *Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms*, Wiley Eastern Limited, New Delhi, 1999.
- T. L. Gilchrist, *Heterocyclic Chemistry*, Pearson Education, 2008.
- T. Eicher, S. Hauptmann and A. Speicher, *The Chemistry of Heterocycles*, Wiley-VCH, 2012.
- G. Brahmachari, *Green Synthetic Approaches for Biologically Relevant Heterocycles*, Elsevier, 2014.
- I. Meyers, *Heterocycles in Synthesis*, John Wiley & Sons, 1974.
- A. R. Katritzky, *Comprehensive Heterocyclic Chemistry*, Elsevier Book series.
- I. Hassner Namboothiri, *Organic Syntheses Based on Name Reactions*, 3rd Edn, Elsevier, 2012.
- L. Kürti and B. Czakó, Strategic *Applications of Named Reactions in Organic Synthesis: Background and Detailed Mechanisms*, Elsevier Academic Press, 2005.
- Z. Wang, *Comprehensive Organic Name Reactions and Reagents*, Wiley-VCH, 2009.
- G. Brahmachari, *Organic Name Reactions: A Unified Approach*, Narosa Publishing House Pvt. Ltd., New Delhi, 2012.
- M. B. Smith and J. March, *March's Advanced Organic Chemistry (Reactions, Mechanisms, and Structure),* 5th Edn, John Wiley & Sons, Inc., 2001.
- R. Bruckner, *Advanced Organic Chemistry (Reaction Mechanisms),* Harcourt/Academic Press, 2002.

- J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
- F. A. Carry and R. J. Sundberg, *Advanced Organic Chemistry – Part-A and B*, 5th Edn, Springer, 2007.
- L. G. Wade, Jr. and M. S. Singh, *Organic Chemistry*, 6th Edn, Pearson Education, 2008.
- T. G. Graham and C. B. Fryhle, *Organic Chemistry*, 8th Edn, John Wiley & Sons, 2004.
- J. Moody, *Reactive Intermediates*, Oxford University Press, 1992.
- R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Edn, Pearson Education, 2013.

CHEM 203C: Physical Chemistry Marks: 50, Credit: 4

1. Harmonic Oscillator

Solution of Schrodinger equation of a Harmonic oscillator using the operator method for solution of differential equation; Selection rules for Harmonic oscillator; rigid rotator, step potential and tunneling; elementary discussion of the H-atom solution; Checking the validity of Schrodinger wave equation based on correspondence principle Heisenberg's Uncertainty principle.

2. Kinetics

Introduction, autocatalysis, chain reactions: branched and non-branched kinetic rate equations, Semenov treatment for branched chain reactions; explosion: population explosion, upper and lower ignition/explosion limits; thermal ignition and ignition temperature; chemical oscillation: some models (Lotka, Oregonater and Brusselator); analysis of Lotka and Brusselator model, conditions for oscillation, chemistry of BZ reaction (Brusselator model); theories of unimolecular reactions: Lindemann, Hinshelwood and RRK theory.

3. Photoexcited Processes

Excitation of molecules – Singlet and Triplet states. Radiative and Non-radiative relaxations. Franck-Condon principle. Absorption, emission and excitation spectra – mirror symmetry. Quenching of Fluorescence. Excited state processes – proton transfer, electron transfer and energy transfer. Marcus Theory. Solvent effect in spectroscopy. Solvation dynamics. Non-linear optical processes. Stimulated emission of radiation. Principles of Laser action. Applications of Lasers.

4. Thermodynamics and statistical mechanics

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. Crystal structure

Crystal symmetry, translation, glide plane and screw axis, Bravis lattice, space groups and its determination, stereographic projection, Fourier series, electron density and structure factor, methods for solving the phase problems, Bzones and Fermi level in lattice, concept of particle-hole in conduction process, band theory, theory of conductors, semiconductors and insulators. Diffraction of X-Ray by crystal, Laue and Bragg condition, concept of reciprocal lattice, crystal structure factor, systematic absence, techniques in X-Ray structure determination.

Reference Books:

- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- R. Taylor, *The Chemistry of Fullerenes*, Advanced Series in Fullerenes, Vol 4, World Scientific, Singapore, 1995
- D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.
- B. P. Houdy and M. Lahmani, *Nanomaterials and Nanochemistry*, Springer, London, 2006.
- N. Levine, *Physical Chemistry*, Tata McGraw-Hill, New Delhi, 1978.
- K. Denbigh, *Principles of Chemical Equilibrium*, Cambridge University Press, Cambridge, 1981.
- M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, John Wiley, New York, 1994.
- G. W. Castellan, *Physical Chemistry*, 3rd Edn, Narosa Publishing House, 1995.
- N. A. Gokcen and R. G. Reddy, *Thermodynamics*, Plenum Press, New York, 1996.
- G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall, India, 1997.
- P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.

- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.
- G. D. Mahan, *Many Particle Physics*, Kluer Academy, Plenum Publisher, 2000.
- Charles Kittel, *Introduction to Solid State Physics*, 4th Edn, John Wiley & Sons, New York.
- P. A. Cox, *The Electronic Structure & Chemistry of Solids*, Oxford University Press, Oxford, 1987.
- M. F. C. Ladd and R. A. Palmer, *Structure Determination by X-ray Crystallography*, 3rd Edn, Plenum Press.
- X. Clegg, *Crystal Structure Determination*, Oxford University Press, Oxford, 2005.

Practical Paper

CHEM 204C(PR): Inorganic Chemistry Practical Marks: 50, Credit: 4

1. Synthesis and Characterization of Inorganic and Coordination Compounds

A. tris(acetylacetonato) complexes of manganese(III), aluminium(III), iron(II), copper(II), vanadium(III/IV)

B. Hexaminecobalt(III)chloride,

C. Polynuclear clusters reported in literature.

D. Copper(II) biguanide.

E. Mn_{12} Acetate Single Molecule Magnet.

F. Mixed valence complex of Mn(III/IV).

G. Preparation of copper glycine complex- cis/trans bis(glycinato)copper (II).

H. Preparation of N,N-bis(salicyldehyde)ethylenediamine, Co(salen), Mn(salen). Selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands.

I. Any suitable compound reported in literature time to time.

2. FT-IR and UV-vis spectral assignment of synthesized metal complexes

3. Growing of **single crystals**

CHEM 205C(PR): Physical Chemistry Practical Marks: 50, Credit: 4

- The rate constant of hydrolysis of an ester/ ionic reaction in a micellar media.
- To verify Ostwald dilution law and determine the Ka of a weak acid.
- To determine the rate constant and salt effect on the rate constant of decomposition of $K_2S_2O_8$ by KI.
- To determine the composition of a mixture of acetic acid, sodium acetate and ammonium acetate by conductometry.

Semester III (Total Marks-300, Credit-24)

Theoretical Papers

CHEM 301C: Inorganic Chemistry Marks: 50, Credit: 4

1. Inorganic Photochemistry

Introduction to inorganic photochemistry, photophysical and photochemical process. Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing, quantum yield, decay fluorescence. Fluorescence quenching, Stern-Volmer equation. Photochemical process: photo substitution and photoelectron transfer reactions in Co, Cr, Ru and Rh complexes. Photosensitization, quenching, charge and energy transfer, prompt and delayed reactions, excimer structure, substitution, fragmentation, isomerisation, exchange and redox reactions; chemiluminescence, photochromism; photochemistry using laser beams; chemical actinometry and determination of quantum yield, inorganic photochemistry in biological processes and their model studies; applications of photochemical reactions of coordination compounds - synthesis and catalysis, solar energy conversion and storage.

2. Magnetochemistry

Basic principles of magnetism, Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, Russell-sander's terms, Magnetic properties and coordination compounds. Magnetic properties of first transition series metal ions, lanthanides and actinides, Lanthanide and actinide contractions and their consequences. Basic concept of Single Molecule Magnets (SMM), properties and examples of SMMs.

3. Inorganic Reaction Mechanism

Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Energy profile diagram of ligand substitution reactions-associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ($\Delta S^{\#}$, $\Delta H^{\#}$, $\Delta V^{\#}$), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy

relation (LFER) etc. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-Condon principle (non mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalyzed substitution reactions.

4. Concepts of Supramolecular Chemistry

New horizon and scientific/technological landscape, building block, atomic and molecular valences, supramolecular orbitals, pallet of non-covalent forces and harnessing them, supramolecular arrays, structure directed synthesis, crystal synthesis, deliberate isolation of different functional materials.

5. Environmental Chemistry

Elements of environment, pollution and pollutants, biodiversity, sustainable ecosystem Air pollution: primary pollutants (CO_2, NO_2, SO_2, HCs, VOCs), photochemical smog, SPM, greenhouse effect, ozone hole and generation of ozone in the atmosphere, El Nino Water pollution: organic and inorganic pollutants, radioactive materials, thermal pollutants; Ground water pollution/arsenic contamination, waste water treatment, water quality.

Soil pollution: waste classification and disposal, solid waste management, detoxification of toxic wastes; radioactive pollution, noise pollution and health Energy resources: conventional and non-conventional energy sources, sustainable development Environmental management: Sectoral examples- thermal power plants, bioparks, chemical industries, textile industries, tannaries, food processing industry, aquaculture projects.

Reference Books

- G. A. Jefferey and W. Saenger, *Hydrogen Bonding in Biological Structures*, Springer, Berlin, 1991.
- 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.
- W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.
- K. Rurack and R. Martinez-Manez (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials*, John Wiley & Sons, Hoboken, New Jersey, 2010.
- E. R. T. Tiekink and J. Zukerman-Schpector (Eds), *The Importance of Pi-Interactions in Crystal Engineering: Frontiers in Crystal Engineering*, 1st Edn, John Wiley & Sons, Chichester, 2012.
- W. Adamson and P. D. Fleischauer (Eds.), *Concept of Inorganic Photochemistry*, Wiley, New York, 1975.

- G. L. Geoffroy and M. S. Wrighton, *Organometallic Photochemistry*, Academic Press, New York, 1970.
- R. Hollebone, C. H. Langford and N. Serpone, *Inorganic Photochemistry, Coord. Chem. Rev.*, 1981, 39, 181.
- F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, New York, 1967.
- D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.
- J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, V; Molecule-based Magnets*, Wiley-VCH, Weinheim, 2005.
- F. E. Mabbs and D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Publications, New York, 2008.
- R. Winpenny (Ed), *Single-Molecule Magnets and Related Phenomena*, Structure and Bonding Series, Vol 122, Springer, Berlin, 2010.
- D. Gatteschi, R Sessoli and J. Villain, *Molecular Nanomagnets*, Oxford University Press, Oxford, 2006.
- R. Hilzinger and W. Rodewald, *Magnetic Materials*, Wiley, New York, 2013.

CHEM 302C: Organic Chemistry Marks: 50, Credit: 4

1. Synthetic Methodology and Advance Organic Synthesis

Organoboron compounds: Hydroboration reaction and synthetic application of its applications organobroranes. Reactions of organoboranes, isomerisation of organoboranes, formation of carbon-carbon bonds, formation of aldehydes, ketones, trialkylcarbinols, reactions of alkenylboranes and trialkylalkynyl borates, free-radical reactions of organoborane.

Organophosphorus compounds: Chemistry of organophosphorus compounds, phosphorus ylids and chiral phosphines.

Organosulphur compounds: Chemistry of organo sulphur compounds, sulphur stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylids, chiral sulphoxide.

Organosilicon compounds: Synthetic uses of silyl ethers, silylenol ethers, TMSCl, TMSI, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acylsilanes; Brook rearrangement, silicon Baeyer Villiger rearrangement.

2. Green Chemistry and Nanoscience

Green Chemistry: Twelve principles of Green Chemistry, Green synthetic methods, catalytic methods, organic synthesis in aqueous media, Ionic liquid, supercritical fluids and microwave. Solvent-free organic reactions.

Nano Science: The nano world (general definition, philosophy), Recent advances in nanomaterials synthesis and characterization, nano-bio interaction and nanomaterials as a drug delivery agent.

3. Natural Product-I

Alkaloids: Structural types; structure elucidation, reactions and synthesis of representative examples (atropine, papaverine, quinine, morphine, camptothecin)

Terpenoids: Isoprene rule, structure elucidation and synthesis of representative examples of acylic, monocylic and bicyclic monoterpens. Structural types; general introduction to sesqui, di- and tri- terpenoids.

4. Organometallic Chemistry of Transition Elements

Application of transition metals in organic synthesis – preparative, structural and mechanistic aspects; Davies rule, catalytic nucleophilic addition and substitution reactions; coupling reaction – Heck, Stille, Suzuki coupling, Ziegler Naata reaction; olefin metathesis; Tebbe's reagent, Pauson-Khand reactions; Volhsrdt co-trimerisation, functional organometallic compounds; use of non-transition metals- Indium, tin, zinc in organic synthesis.

Reference Books

- M. Schlosser and K. Smith, *Organoboron Chemistry*, Wiley-VCH, 2013.
- M. G Davidson, K. Wade, T B Marder and A.K Hughes (Eds), *Contemporary Boron Chemistry*, Royal Society of Chemistry, 2000.
- B. Marciniec, *Progress in Organosilicon Chemistry*, Taylor & Francis, 1995.
- N. Auner and J. Weis (Eds), *Organosilicon Chemsitry III: From Molecules to Materials*, Wiley-VCH, 1998.
- G. H. Whitham, *Organosulfur Chemistry*, Oxford University Press, 1995.
- R. J. Cremlyn, *An Introduction to Organosulfur Chemistry*, Wiley-VCH, 1996.
- R. Engel, *Handbook of Organophosphorous Chemistry*, CRC Press, 1992.
- D. Quin, *A Guide to Organophosphorus Chemistry*, Wiley-VCH, 2000.
- D. W Allen, D. Loakes and J. C Tebby (Series Eds), *Organophosphorous Chemistry*, RSC Book Series.

- P. G. M. Wuts and T. W. Greene, *Greene's Protective Groups in Organic Synthesis*, 4th Edn, Wiley-VCH, 2006.
- E. J. Corey and X.-M. Chelg, *The Logic of Organic Synthesis*, John Wiley & Sons, 1995.
- P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice,* Oxford University Press, 2000.
- P. T. Anastas (Series Ed.), *Handbook of Green Chemistry*, Wiley-VCH Book Series.
- J. H Clark (Series Editor-in-Chief), *RSC Green Chemistry*, Royal Society of Chemistry Book Series.
- V. K. Ahluwalia and K. Kidwai, *New Trends in Green Chemistry*, Springer, 2004.
- R. A. Sheldon, I. Arends, and U. Hanefeld, *Green Chemistry and Catalysis*, Wiley-VCH, 2007.
- A. K. Kruthiventi and M. Doble, *Green Chemistry and Engineering*, Academic Press, 2007.
- G. Brahmachari, *Green Synthetic Approaches for Biologically Relevant Heterocycles*, Elsevier, 2014.
- V. K. Ahluwalia, *Green Chemistry: Environmentally Benign Reaction*, Ane Books, 2006.
- V. M. Kolb, *Green Organic Chemistry and its Interdisciplinary Applications*, CRC Press, 2016.
- S. K. Sharma and A. Mudhoo, *Green Chemistry for Environmental Sustainability*, CRC Press, 2010.
- P. Dicks, *Green Organic Chemistry in Lecture and Laboratory*, CRC Press, 2011.
- S. A. Henrie, *Green Chemistry Laboratory Manual for General Chemistry*, CRC Press, 2015.
- R. C. Mehrotra, *Organometallic Chemistry*, New Age International, 2007.
- G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, oxford University Press, 2010.
- D. Gupta, *Basic Organometallic Chemistry: Concepts, Syntheses and Applications*, Universities Press, 2011.
- D. Astruc, *Organometallic Chemistry and Catalysis*, Springer, 2007.

CHEM 303C: Physical Chemistry **Marks: 50, Credit: 4**

1. Group Theory-II

Great Orthogonality Theorem- statement and interpretation. Proof of its corollaries. Character table and its construction. Number of times an irreducible representation occurs in a reducible one. The reduction of reducible representations. Notation of irreducible representations. Representations and quantum mechanics. The invariance of Hamiltonian operator under symmetry transformations. Direct product representation. Molecular vibrations. Symmetry species of the vibrational mode. Selection rules for Infra-red and Raman spectra. Crystal field splitting.

2. Surface Chemistry and Bio-Physical Chemistry

Surface tension, curved surfaces, Young-Laplace and Kelvin equations. Adsorption on solids, micelles reverse micelles, microemulsion, Thermodynamics of micellization, Application of micelles and microemulsion. Hydrophobic hydration, micelle formation, hydrophobic interaction, stabilization and denaturation of protein. Water structure alternation theory of denaturation of protein, protein–lipid interaction, Transport of ions and small molecules through membranes. Ion channels.

3. Macromolecules

Introduction; Carothers' equation, average molecular weights and their determination; kinetics of addition and condensation polymerization, 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. Electric and Magnetic properties of Matter

Molecular response parameters – Polarizability. Dispersion forces. Bulk electrical properties – Permittivity and Susceptibility. Refractive index. Dielectric relaxation. Optical activity and Circular birefringence. Conduction in dielectrics. Magnetic susceptibility. Paramegnetism and Diamagenetism. Vector potential and current density. Shielding constants. The g-value. Spin-spin coupling and Hyperfine Interactions.

5. Thermodynamics of irreversible processes

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 scaler and one vector force, illustrations; Saxen's relations in connection with electrokinetic phenomena and their proof using Onsager reciprocity relations, stationary states: variation of entropy production with time, Prigogine's criterion for establishment of stationary state, applicability of Le Chateliar's principle on stationary states.

Reference Books:

- 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. 2007.
- D. M. Bishop, *Group Theory and Chemistry*, Oxford University. Press, 1993.
- J.Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.
- D. P. Woodruff and T. A. Delchar, *Modern Techniques of Surface Science*, Cambridge University Press, Cambridge, 1988.
- W. Adamson, *Physical Chemistry of Surfaces*, John Wiley & Sons, New York, 1990.
- H. -J. Butt, K. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, Wiley-VCH, 2003.
- H. Clint, *Surface Chemistry*, Blackie and Son Ltd, 1992.
- C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley & Sons, Inc, New York, 1961.
- W. Billmeyer, *Text Book of Polymer Science*, 2nd Edn, Wiley-Interscience, New York, 1971.
- S. Mishra, *Introductory Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.
- P. Ghosh, *Polymer Science and Technology of Plastic and Rubber*, Tata McGraw-Hill Publishing Company Limited. 2008.
- S. F. Sun, *Physical Chemistry of Macromolecules: Basic Principles and Issues*, John Wiley & Sons, New York, 1994.
- A.J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.
- J. F. Böttcher, *Theory of Electric Polarisation*, Vols 1 and 2, Elsevier Scientific Publishing Co, New York, 1973.
- W. Davies, *The Electric and Magnetic Properties of Molecules*, 1967.
- K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, New Age International (P) Limited, Publishers, India, 2007.

Practical Paper

CHEM 304C(PR): Organic Chemistry Practical Marks: 50, Credit: 4

1. Separation, purification and identification of organic compounds in binary mixture (two solids) using chemical tests and TLC. (At least 6 samples are to be worked up during the lab session).

2. Chromatographic Separation Techniques and Spectroscopic Studies of Model Compounds

A: Chromatographic separation techniques: Thin layer chromatography, paper chromatography, column chromatography separation of binary mixture of organic compounds and choice of illutent.

B: Recording of electronic spectra of different types of compounds in water, in ethanol or in other suitable solvents, Determination of absorption maxima and molar extinction coefficient values.

CHEM 306C(PR): Physical Chemistry Practical Marks: 50, Credit: 4

1. To determine the concentrations of a strong and a weak acid in a given mixture by potentiometry.
2. To determine the formal potential of Fe(III)/ Fe(II) couple by potentiometry.
3. To determine the dissociation constant of Phenolphthalein indicator by spectrophotometry.
4. To study the kinetics of alkaline hydrolysis of crystal violet by spectrophotometry.

CHEM 305 EID: Marks: 50, Credit: 4

1. Structure and Properties of Organic Molecule

Nature of bonding in aliphatic, alicyclic, aromatic and heterocyclic compounds; bond length, bond strength, bond angle and their variations in compounds with sp^3, sp^2 and sp hybridized carbon atoms; orbital pictures of methane, ethane, ethene, ethyne, allene and benzyne; delocalised bonds, resonance, steric inhibition of resonance, hyperconjugation, tautomerism, aromaticity, Huckel's rules, aromatic, nonaromatic and antiaromatic compounds, non-benzenoid aromatic compounds, Huckel's rule. Formation, structure, stability and reactions of classical and non-classical carbocations, carbanions, free radicals, arynes, ylides, carbenes and nitrenes.

2. Atomic Structure

Bohr's model, Sommerfeld's extension, de Broglie's wave particle duality; Heisenberg's uncertainty principle and Schrödinger's equation (qualitative); significance of ψ and ψ^2; radial density, angular probability, characteristics of s-/p-/d-orbital, Aufbau principle, Pauli's exclusion/antisymmetry principle (statement and implication), Hund's rules, Slater's rules, quantum defect.

Mendeleev-Seaborg's periodic table: basis and possible extension; periodic properties: atomic radius, ionic radius, covalent radius, van der Waals radius, ionization energy, electron affinity, electronegativity and its different scales, orbital/group electronegativity, ionic potential, diagonal relationship, work function; aperiodicity.

3. Kinetic Theory of Gases

Idea of distribution functions, properties of gamma functions, Maxwell's speed and energy distributions in one-, two- and three- dimensions, distribution curves, different types of speeds and their significance, principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases.

Reference Books

- 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*, Mercel Dekker, New York, 1974.
- J. J. Li, *Name Reactions: A Collection of Detailed Reaction Mechanisms*, Springer, 2014.
- G. Brahmachari, *Organic Name Reactions: A Unified Approach*, Narosa Publishing House Pvt. Ltd., New Delhi, 2012.
- M. B. Smith and J. March, *March's Advanced Organic Chemistry (Reactions, Mechanisms, and Structure)*, 5th Edn, John Wiley & Sons, Inc., 2001.
- R. Bruckner, *Advanced Organic Chemistry (Reaction Mechanisms)*, Harcourt/Academic Press, 2002.
- J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
- F. A. Carry and R. J. Sundberg, *Advanced Organic Chemistry – Part-A and B*, 5th Edn, Springer, 2007.
- L. G. Wade, Jr. and M. S. Singh, *Organic Chemistry*, 6th Edn, Pearson Education, 2008.

- J. Moody, *Reactive Intermediates*, Oxford University Press, 1992.
- R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Edn, Pearson Education, 2013.
- J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorgnic Chemistry: Principles of Structures and Reactivity*, 4th Edn, Pearson, New Delhi, 2006.
- F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley & Sons, Inc, New York, 1999.
- P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006.
- P. C. Rakshit (Revised by S. C. Rakshit), Physical Chemistry, Sarat Book Distributers, Kolkata.
- P.W. Atkins and Julio De Paula, Physical Chemistry, Oxford University Press, Oxford.
- Pahari & Pahari, Problems on Physical Chemistry,New Central Book Agency (P) Ltd.
- S. Glasstone, Text Book of Physical Chemistry, Macmillan & Company Ltd, London.
- D.A. Mc-Quarie and J .D. Simon, Physical Chemistry: A Molecular Approach, Viva Book Pvt. Ltd.
- A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill Publishing Company Ltd.
- P. T. Matthews, Introductory Quantum mechanics, Mcgraw-Hill.
- L.I. Schiff, Quantum Mechanics, McGraw Hill International Edition.
- F.A. cotton, Chemical Application of Group Theory, Interscience Publishers, New York (1963)
- J.O'M Bockeris, A.K.N Reddy and M.G. Aldeco, Modern Electrochemistry, Published by Springer.
- Samuel Glasstone, An Introduction to Electrochemistry, East West Press Private, Limited.
- Berry, Rice and Ross, Physical Chemistry, Oxford University Press.

Semester IV (Total Marks-300, Credit-24)

Special Theoretical Papers

CHEM 401E: Marks: 50, Credit: 4

Inorganic Special

1. Studies and Applications of Lanthanoids and Actinoids

Spectral and magnetic properties, use of lanthanoid compounds as shift reagents, Modern methods of separation of lanthanoids and actinoids, Organometallic chemistry applications of lanthanoid and actinoid compounds in Industries.

2. Isopoly and Heteropoly Acids and Salts

Isopoly and Heteropoly acids and salts of V, Mo and W: pH dependence, Structures of isopoly and heteropoly anions. Keggin's structure.

3. Host-guest Chemistry

Synthesis and structures of crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarene, Cyclodextrins, Cyclophanes, Cryptophanes, Carcerands and hemicarcerands, Host-guest interactions, Preorganisation and complimentarity, Lock and key analogy, Binding of cationic, Anionic, Ion pair and neutral guest molecules.

4. Supramolecular Veracities

Self-assembly molecules: Design, Synthesis and Properties of the molecules, Self-assembly by H-bonding, Catenanes, Rotaxanes, Dendrimers and Supramolecular gels. Relevance of supramolecular chemistry to mimic biological system. supramolecular arrays: ribbon. Ladder, rack, braded, grid. Dendrimers.

5. Molecular Devices

Molecular Electronic devices, Molecular wires, Molecular rectifiers, Molecular switches and Molecular logic gates. Examples of recent developments in supramolecular chemistry from current literature, molecular recognition.

6. Corrosion

Different types of corrosion; influence of environment; Evans diagram, Pourbaix diagram; corrosion rate measurements; Stern Geary equation; mixed potential theory and prevention of corrosion.

7. Mössbauer Spectroscopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (2) Sn^{2+} and Sn^{4+} compounds nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Reference Books

- E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Mehdi, *Inorganic Chemistry, Principles of Structure and Reactivity*, 4th Edn, Pearson, 2006.
- F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, Wiley, 2007.
- C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, 4th Edn, Pearson, 2012.
- G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 1997.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.
- R. Martinez-Manez and K. Rurack (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials*, John Wiley & Sons, Hoboken, New Jersey, 2010.
- J . M. Lehn, *Supramolecular Chemistry - Concepts and Perspectives*, Wiley-VCH, 1995.
- P. D. Beer, P. A. Gale and D. K. Smith, *Supramolecular Chemistry*, Oxford University Press, 1999.

Organic special

1. Techniques of Chemical Separation

Principles, classification, experimental set up, special features, mechanism of separation procedures, advantages and disadvantages, and applications (analytical and/or industrial) of the following separation techniques.

- **Chromatography:** Fundamentals, dynamics, plate theory, resolution of mixtures. Absorption chromatography-chemical constitution and chromatographic-behaviour, affinity chromatography and chiral chromatography. Partition chromatography-liquid-liquid and reverse phase partition chromatography, paper chromatography, thin layer chromatography (TLC) and ion pair chromatography.
- **Gas chromatography (GC):** Plate theory, gas-solid and gas-liquid chromatography, HPLC. Super critical fluid chromatography, gel permeation chromatography and molecular sieves. Hyphened technique. GC-MS and its applications.
- **Electrochromatographic techniques:** Curtain electro-chromatography, reverse osmosis and electro-dialysis and their applications in desalination of water, separation of biomolecules by electrophoresis, capillary electrophoresis.
- **Solvent extraction:** Extraction equilibria, partition coefficient and extraction coefficient, extraction by chelation and solvation; solid-phase extraction (SPE), supramolecular extraction with crown ethers, cryptands and rotaxenes.

2. Hetercyclic Chemistry-II

Fused systems: nomenclature. Synthesis and reactions of

(i) Azoles: pyrazole, imidazole, oxazole and thiazole.

(ii) Diazine: pyridazine, pyrimidine and pyrazine.

(iii) Purine, pteridine and folic acid.

ANRORC and Vicarious nucleophilic substitutions in heterocycles.

3. Natural Product-II

Structure,synthesis and reacations of flavonoids and coumarins. Reaction and synthesis of steroids (cholesterol, bile acid, testosterone, estrone, progesterone).Structure and synthesis of porphyrins (haemoglobin, chlorophyll). Structure and synthesis of prostaglandins (PGE_2, $PGF_{2\alpha}$).

4. Medicinal Chemistry

Different types of drugs. Drug-receptor interactions, mechanisms of drug action. Drug designing and synthesis. Concepts of LD_{50} and ED_{50}. Structure-Activity Relationship (SAR) and Quantitative Structure Activity Relationship (QSAR) with special reference to antimalarials, Antibiotics: Cell wall biosynthesis, inhibitors, β-lactam rings, synthesis of penicillin;synthesis and mode of action of sulphonamides, nalidixic acid, norfloxacin, aminosalicyclic acid, ethinamide, fluconazole, chloroquin and premaquin; Antidiabetic drugs: insulinsensitizers (biguanides, thiazolidinediones), secretagogues (sulfonylureas, nonsulfonylurea secretagogues, alpha-glucosidase inhibitors, peptide analogues (injectable incretin mimetics, injectable amylin analogues); *Cardiovascular drugs*: Introduction to cardiovascular diseases, synthesis and mode of action of statins, amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil and methyl dopamine, antibiotics, anticholenergics and CNS active drugs. Vitamins: vitamin-Bcomplex, vitamin C, vitamin K.

Reference Books

- 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*, Academic Press, 1970.
- S. Sankararaman, *Pericyclic Reactions – A Textbook,* Wiley-VCH Verlag, 2005.
- I. Fleming, *Pericyclic Reactions*, Oxford University Press, 1996.
- F. Vögtle, *Supramolecular Chemistry: An Introduction*, John Wiley & Sons, 1991.
- M. Lehn, *Supramolecular Chemistry: Concept and Perspectives*, Wiley-VCH, 1995.
- P. J. Cragg, *Supramolecular Chemistry*, Springer, 2010.
- H. -J. Schneider and A. Yatsimirsky, *Principles and Methods in Supramolecular Chemistry*, Wiley-VCH, 1999.
- Ariga T. Kunitake, *Supramolecular Chemistry - Fundamentals and Applications*, Springer, 2006.
- J. C. Gallagher and C. MacDougall, *Antibiotics Simplified*, 3rd Revised Edn, Jones and Bartlett Publishers, Inc. 2013.
- C. Walsh, *Antibiotics: Actions, Origins, Resistance*, Wiley-VCH, 2016.
- S. Sánchez and A. L. Demain, *Antibiotics: Current Innovations and Future Trends*, Caister Academic Press, 2015.
- B. Testa and U. A. Meyer, *Antidiabetic Agents: Recent Advances in their Molecular and Clinical Pharmacology*, Acdemic Press, 1996.
- K. Chatterjee and E. J. Topol, *Cardiac Drugs*, Jaypee Brothers Medical Pub., 2013.

- W. H. Frishman and D. A. Sica, *Cardiovascular Pharmacotherapeutics*, 3rd Edn, Cardio Text, 2011.
- A.Rahman and M. I. Choudhary, *Frontiers in Cardiovascular Drug Discovery*, Bentham Publications, 2010.
- S. Quideau, *Chemistry and Biology of Ellagitannins*, World Scientific Publishing Co., 2009.

Physical Special

1. Approximate Methods and their Applications

Variation theorem, linear variation method, Applicability of variation method to excited states. Time-independent perturbation theory for nondegenerate states, Perturbation of a two-level system, Many level systems, Degenerate perturbation theory and their applications, Eckert's Theorem. Hydrogen and Helium atoms. Hellman-Feynman and Viral Theorems. Time-dependent perturbation theory, Rabi Oscillation, Many level system; the variation of constants, the effect of slowly switched constant perturbation, The effect of oscillating perturbation, Transition rates to continuum, Radiationmatter interaction. Fermi Golden rule, Einstein transition probabilities, lifetime and energy uncertainty.

2. Spin and Many Electron Wave functions

Introduction to spin. Operator algebra for spin. Construction of matrix representation of spin operators, Eigenvalues and Eigen functions of spin operators. Non-relativistic wave function for Hydrogen atom. Many-electron wave functions- examples with 2 and 3 electron systems, Slater determinants. Projection Operators. Parity Operator and Pauli Principle, The Pauli exclusion principle. Introduction of core, Coulomb, and exchange integrals with their properties- example of He atom.

3. Theory of Many-electron Systems and their Applications

The Born-Oppenheimer approximation, Hartree self consistent field method, Koopman's theorem, Hartree-Fock method for many-electron systems. Coulomb operators, Exchange operators, Coulomb and Fermi hole, Restricted and unrestricted Hartree-Fock calculations, The Roothan equation. Correlation energy, Basis sets for electronic structure calculations. Spin-orbit interaction, The Condon-Slater rules.

4. Density- Functional and Semi empirical Methods in Quantum Chemistry

Introduction to density functional, Hohenberg-Kohn variation theorem, Kohn-Sham equations, Exhange-correlation energy, Local density approximation, Generalized gradient approximation. Semi empirical MO treatments of Planar Conjugated Molecules, The Free electron MO method, The Huckel and Extended Huckel MO method, The Pariser-ParrPople method, General semi empirical MO methods.

Reference Books:

- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- R. Taylor, *The Chemistry of Fullerenes*, Advanced Series in Fullerenes, Vol 4, World Scientific, Singapore, 1995.
- D. A. Mc-Quarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.
- N. R. Rao, A. Müller, A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications.*
- B. P. Houdy and M. Lahmani, *Nanomaterials and Nanochemistry*, Springer, London, 2006.

CHEM 402E: Marks: 50, Credit: 4

Inorganic Special

1. Inorganic Materials

Design and synthesis of inorganic materials, requirements and constraints, combination properties of composites, functional materials, active materials; solid state reactions for synthesis of inorganic materials: ceramic methods, precursor method and sol-gel synthesis, physical and chemical vapour depositions; carbides, nitrides, structural and functional ceramics, intermetallics; intrinsic and extrinsic properties: electrical, optical and magnetic properties; ceramic superconductors, magnetic ceramics secondary building unit (SBU), functional materials: conducting, superconducting, magnetic, non-linear, porous, luminous, liquid crystals, catalysts, molecular and electronic devices, biosensors, bio mineralization.

2. Synthesis, Structure, Properties, Structure-property Correlations and Potential Applications of Crystalline Inorganic Solid State Materials

Superconductors – (Ba,K)BiO_3, Cuprates, LnFeAsO, MgB_2, CaC_6

CMR materials – $La_{1-x}Sr_xMnO_3$

Ferroic compounds – $BaTiO_3$, $PbTiO_3$, $Bi_4Ti_3O_{12}$, $SrRuO_3$

Photoluminescent materials – Lanthanoid compounds Porous materials – zeolites, AlPO, MeAlPO, SAPO.

Organic-inorganic hybrid materials – Ruddlesden-Popper $(RNH_3)_2A_{n-1}MX_{3n+1}$ metal halides, MOF compounds.

Ionic Conductors – NASICON, AgI, $NaAl_{11}O_{17}$

Thermoelectric materials – $NaxCoO_2$, $AgSbTe_2$, $CoSb_3$, $Y_{14}MnSb_{11}$

Compounds for intercalation and redox reactions – $LiCoO_2$, $LiVS_2$, NASICON

3. Chemistry of Elements and Their Compounds

Elements – structural versatility and related properties; compounds – design, benign, modular and reticular syntheses, isolation, characterization, solution structure, molecular aggregate, crystalline architecture, spectral, magnetic and catalytic properties and application in chemistry, biology and materials science.

Non-transition and transition metal ion homoleptic/heteroleptic and homonuclear/heteronuclear complexes of different dimensions with varied mono- and polydentate blockers containing carbon,

nitrogen, phosphorus, chalcogen, halogen donors with/without mono-/polydentate bridges and counter ions.

Mono- and polynuclear compounds of lanthanoid and actinoid ions stressing on choice of different multidentate chelators and congregators with special emphasis on electric, magnetic, conducting, superconducting and fluorophoric behaviours.

4. Metallomesogens

Basic concepts, synthetic strategies, characterization and applications.

5. Preparative Methods

Solid state reaction, chemical precursor method, coprecipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion-exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis; High pressure synthesis.

6. Methods of Single Crystal Growth

Solution growth; Melt Growth-Bridgeman, Czochralski, Kyropoulus, Verneuil; Chemical Vapour Transport; Fused Salt Electrolysis; Hydrothermal method; Flux Growth.

7. LASER spectroscopy in Inorganic Complexes

Introduction, Fundamental principles, Laser sources and method, Tunable and single frequency Laser operation, Laser pulses –time and intensity dependent phenomena, Laser techniques such as Fluorescence and Excitation Line Narrowing (FLN and ELN) spectroscopy, Spectral hole burning, Photon echo measurement, two photon and single molecule spectroscopy

Reference Books

- C. N. R. Rao and J. Gopalakrishnan, *New directions in Solid State Chemistry*, Cambridge University Press: Cambridge, 1997.
- A. K. Cheetham, *Solid state chemistry: compounds*, Oxford University Press, Oxford, 1992.
- J. N. Lalena and D. A. Cleary, *Principles of Inorganic Materials Design*, Wiley, New York, 2010.
- J. Maier, *Physical Chemistry of Ionic Materials: Ions and Electrons in Solids*, Wiley: New York, 2004.
- E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Mehdi, *Inorganic Chemistry, Principles of Structure and Reactivity,* 4th Edn, Pearson, 2006.
- F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry,* 6th Edn, Wiley, 2007.
- C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry,* 4th Edn, Pearson, 2012.

Organic Special

1. Supramolecular Chemistry

Factors leading to binding (noncovalent interactions). New molecular receptors: crown ethers, cryptands, cyclophanes, siderophores, cyclodextrin, and their application in specific recognition processes. Supramolecular reactivity and catalysis, switching devices. Self-assembly of supramolecular aggregates, principles of gene synthesis, catalytic antibodies, molecular channels, transport processes and carrier design. Supramolecular devices and nanotechnology. Supramolecular photochemistry**.**

2. Asymmetric Synthesis-II

Principles and newer methods of asymmetric synthesis (including enzymatic and catalytic nexus); enantio- and diastereoselective synthesis;reactions of enolates (α-substitution); addition to C=C double bonds (electrophile-induced cyclisation, iodolactonisation, hydroboration, conjugate additions); asymmetric hydrogenation with special reference to Ru-BINAP catalysts; asymmetric epoxidation with special reference to Sharpless and Jacobsen epoxidation; asymmetric aldol reactions, asymmetric Michael reaction; Few important industrial applications of asymmetric synthesis.

3. Photochemistry and Free Radical

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomeriation stereomutation Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pimethane rearrangement, photochemistry of arenes, Photoreaction in solid state, Barton reaction, Hofmann-Loffler-Freytag reaction. Method of generation and detection (ESR) of radicals, radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, autooxidation.

4. Oxidation and Reduction of Functional Group

Oxidation reactions:

Oxidation of hydrocarbons, oxidation of alcohols by various reagents, and methods, oxidation of carbon-carbon double bonds to diols and epoxides, Woodward and Prevost Reaction, synthetic reactions of epoxides, diastereo-selective epoxidation of homoallylic alcohols, photosensetised oxidation of alkenes, oxidation of ketones to α,β-unsaturated ketones. Oxidation with ruthenium tetroxide, iodobenzene diacetate, and thallium(III) nitrate.

Reduction reactions:

Catalytic hydrogenation - the catalyst, selectivity of reduction, reduction of functional groups, stereochemistry and mechanism, homogeneous hydrogenation. Reduction by dissolving metals-reduction with metal and acid, reduction of carbonyl compounds, Birch Reduction. Reduction by hydride transfer reagents-aluminium alkoxides, LAH and $NaBH_4$, lithiumhydridoalkoxyaluminates, lithiumaluminiumhydride-aluminiumchloride reagents, diisobutylaluminiumhydride, sodium cyanoborodydride, trialkylborohydrides. Other methods - desulphurisation of thioacetals, diimides, low-valent titanium species, trialkyltinhydrides.

Reference Books

- O. M. Anderson and K. R. Markham, *Flavonoids: Chemistry, Biochemistry and Applications*, CRC Press, Taylor & Francis, 2006.
- S. K. Talapatra and B. Talapatra, *Chemistry of Plant Natural Products*, Springer, 2012.
- S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, *Chemistry of Natural Products*, Narosa Publishing House, New Delhi, 2005.
- M. M. M. Pinto, *Chemistry of Love and Sex*, Wiley-VCH, 2012.
- D. B. Gower, *Steroid Hormones*, Year Book Medical Pub., 1979.
- X. -T. Liang and W.-S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.
- P. Manitto, *Biosynthesis of Natural Products*, Ellis Horwood Ltd., 1981.
- T. Hudlicky and J. W. Reed, *The Way of Synthesis*, Wiley-VCH, 2007.
- D. Bogdal, *Microwave-assisted Organic Synthesis*, Elsevier, 2005.
- G. Brahmachari, *Room Temperature Organic Synthesis*, Elsevier, 2015.
- G. Brahmachari, *Green Synthetic Approaches for Biologically Relevant Heterocycles*, Elsevier, 2014.
- B. C. Ranu and A. Stolle, *Ball Milling Towards Green Synthesis: Applications, Projects, Challenges*, Royal Society of Chemistry, 2014.
- R. Cella and H. A. Stefani, *Ultrasonic Reactions, In: Green Techniques for Organic Synthesis and Medicinal Chemistry* (Eds W. Zhang and B. W. Cue), John Wiley & Sons, Ltd, Chichester, UK, 2012.
- K. Tanka, *Solvent-free Organic Synthesis*, 2nd Edn, Wiley-VCH, 2009.
- V. K. Ahluwalia and M. Kidwai, *New Trends in Green Chemistry*, Springer, 2004.

- N. J. Turro, *Modern Molecular Photochemistry*, The Benjamin/Cummings Publishing Co., Inc., 1978.
- R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Academic Press, 1970.
- J. M. Coxon and B. H. Halton, *Organic Photochemistry*, Cambridge University Press, 1974.

Physical Special

1. Excitation of Molecules and Motion in Excited State

Theory of Electromagnetic Radiation. Interaction between Matter and Electromagnetic Radiation – Semi classical treatment using Time-dependent perturbation Theory. Fermi golden rule, Transition probabilities and rates, Spectral shapes. Decoupling of the nuclear and electronic motions in a molecule: Born-Oppenheimer approximation.

2. Rotational, Vibrational and Raman Spectroscopy

Rigid and Non-rigid Rotors. Vibrational spectroscopy – Harmonic and Anharmonic Oscillators. Normal coordinates. Effects of Anharmonicity. Vibration-rotation transitions. Raman and Rayleigh scattering – Classical and Quantum Mechanical treatments. Polarization of scattered light. Rotational and Vibrational Raman spectroscopy. Resonance Raman Effect. Selection rules of rotational, vibrational and Raman spectroscopy. Instrumentation of microwave, IR and Raman spectroscopy.

3. Electronic Spectroscopy

Atomic structure: vector model, spin-orbit coupling, atomic states and term symbols. Many-electron atoms – Hund's rules. Selection rules for atomic electronic transitions. Diatomic molecules – Hund's coupling cases. Rotational and vibrational structures of diatomic electronic transitions. Franck-Condon principle. Dissociation, Photodissociation and Predissociation. Polyatomic molecules – orbitals and electronic states. Chromophores. Vibronic transitions. Spin-orbit coupling and singlet – triplet transitions. Selection rules for molecular electronic transitions. Photoelectron spectroscopy. Rotational structure of some polyatomic electronic transitions. Instrumentation of UV-visible absorption and emission spectroscopy.

4. Spin Spectroscopy – NMR and ESR

Nuclear magnetic moment and response in an external magnetic field. Classical and Quantum Mechanical perspectives of nuclear magnetic resonance (NMR). Bloch equations. Spin-spin and spin-lattice relaxation and spectral shapes. Free induction decay and FT-NMR technique. Chemical shift and nuclear shielding. Spin magnetic moment of electrons and electron spin resonance signal (ESR). The g-factor and hyperfine splitting – interaction between nuclear spin and electron spin. Applications and instrumentation of NMR and ESR. Multi-dimensional NMR spectroscopy. Nuclear quadrupole resonance.

Reference Books

- G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company, Tokyo, 1982.
- W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, Hong Kong, 1986.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- K. M. Sanders, E. C. Constable and B. K. Hunter, *Modern NMR Spectroscopy: A Workbook of Chemical Problems*, Oxford University Press, Oxford, 1993.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd.
- H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.
- 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*. 1989.

CHEM 403E: Marks: 50, Credit: 4

Inorganic Special

1. Solid Electrolytes

Typical Ionic Crystals: Alkali metal halides (vacancy conduction), silver chloride (interstitial conduction); Solid Electrolytes - β-alumina, silver iodide, halide and oxide ion conductors; Application of Solid Electrolytes. Fuel cells: electrochemical power generator (hydrogen-oxygen cell, Solid state Galvanic cell); Thermoelectric Effects: See beck effect; Hall Effect.

2. Metals in Medicine

Metal deficiency and disease; toxicity of mercury, cadmium, lead, beryllium, selenium and arsenic; biological defence mechanisms; chelation therapy; metals used for diagnosis and chemotherapy, platinum complexes as anticancer drugs, Pt-DNA binding, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

3. Atomic X-Ray Spectroscopy

Fundamental principles, Instrument component, X-ray Fluorescence method, X-Ray absorption method, The electron microprobe, Electron spectroscopy for chemical analysis (ESCA), Auger Emission spectroscopy (AES).

4. Atomic Emission Spectroscopy

Introduction, Instrumentation, Typical applications, ICP atomic Fluorescence spectroscopy, Comparison of methods: ICP Vs AAS.

5. Vibrational and Raman Spectroscopy

Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, mode of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes, Theory of Raman spectroscopy, Instrumentation, Sample handling and Illumination, structural analysis , polarization measurements, quantitative analysis , applications of Raman spectroscopy, other types of Raman spectroscopy, Comparison of Raman and Infrared spectroscopy.

6. Surface Characterization by Spectroscopy and Microscopy

Introduction to the study of surfaces, Spectroscopic surface methods, Electron spectroscopy, Ion Spectroscopic techniques, Surface photons spectroscopic methods, Electro- stimulated micro analysis methods, Scanning probe microscopies.

7. Extended X-Ray Absorption Fine Structure (EXAFS) Analysis

EXAF theory- single scattering (SS) and multi scattering (MS) theory, Data analysis using GNXAS approach, GNXAS application to inorganic system, Implication of using GNXAS MS approach for study of biological system.

8. Mass Spectrometry

Molecular mass spectra , Sample flow in mass spectrometer, Inlet sample system , Ion sources , Mass spectrometers, Applications of molecular mass spectrometry, Quantitative application of mass spectrometry, ICP-MS , Secondary Ion Mass Spectrometry (SIMS), Ion Microprobe Mass Analyzer (IMMA).

Reference Books

- D. A .Skoog, F. J. Holler and S. R. Crouch, *Instrumental analysis*, Cengage Learing India Pvt. Ltd., New Delhi, 2007.
- H.H. Willard, L.L. Merritt. Jr. J.A. Dean and F.A. Settle, Instrumental method of analysis (7th edition) Jr (Publisher: CBS Publishers and distributors Pvt .Ltd. (Copyright – wardsworth publishing copy USA .2000)).
- G.D. Christian, Analytical chemistry (6th Edn): (John Wiley and sons Pvt. Ltd. Singapore, 2009).
- G.Currell, Analytical Instrumentation: Performance characteristics and Quality: (John Wiley and sons Pvt. Ltd. 2000) chapter .4.
- Edward I. Soloman and A.B.P. Lever, Inorganic Electronic Structure and Spectroscopy Volume 1, Methodology; (Wiley Interscience Publication, 2013).
- C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, McGraw-Hill, 1994.
- H. Gunther, NMR Spectroscopy, Basic Principles, Concepts and Applications in Chemistry, 3rd Edition, Wiley VCH, 2013.

Organic special

1. Protein, Nucleic acid, Lipid and Co-enzyme Chemistry

Proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, Ramachandran Diagram, forces responsible for holding of secondary structures, α-helix, β-sheets, tertiary structure of protein-folding, quaternary structure, biosynthesis of peptide chain.

Nucleic acids: Chemical synthesis of nucleic acids. Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it.

Lipids: Fatty acids, structure and function of triacylglycerols, glycerophospholipids, properties of lipid bi-layers, biological membranes, fluid mosaic model of membrane structure.

Enzymes: Chemical and biological catalysis, properties of enzymes like catalytic power, specificity and regulation, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis; mechanism of enzyme action: transition state theory,examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease.

2. Bioorganic Chemistry

The molecules of life

Nucleic acids, purine and pyrimidine bases, nucleosides, and nucleotides. Genetic code of life, replication, transcription and translation of DNA, genetic information transfer and heredity. Types of sugars, deoxy sugars, amino sugars and polysaccharides.

Enzymes

Catalytic power of enzymes, specificity and regulation. Nomenclature and classification, extraction (large scale production) and purification of enzymes. Immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology.

Mechanism in biological chemistry:

- Mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxy-peptidase-A.
- Enzyme catalyzed reactions - Examples of nucleophilic displacement on a phosphorus atom, coupling of ATP cleavage to endergenic processes, proton transfer reactions to and from carbon.

- Mechanism of reactions catalyzed by cofactors including coenzyme-A, NAD+, NADH, FAD and thiamin phosphate.
- Chemical synthesis of peptides and proteins. Use of enzymes in organic synthesis.
- Structural analysis of proteins. Protein folding.

Coenzymes and Co-factors:

Vitamins, prosthetic groups epoenzymes, structures and biological functions of coenzyme-A, thiamine pyrophosphate, pyrodoxal phosphate, NAD+, NADP+, FMN, FAD, Coenzyme Q, Lipoic acid, Vitamin -B_{12}.

3. Carbohydrates

Abnormal mutarotation of monosaccharides; use of complexing agents: borates, phosphates and copper compound; synthesis of glycosides; general treatment of polysaccharide chemistry: isolation, purification, hydrolysis, methylation and periodic oxidation, Smith degradation, Barry degradation.

4. CD-ORD-VCD

Chiroptical properties of organic molecules, origin, theory. CD, ORD and VCD principles and applications, haloketone rules, sector rules, helicity rules. Application to biological molecules

Reference Books

- S. Sankararaman, *Pericyclic Reactions – A Textbook*, Wiley-VCH Verlag, 2005.
- M. Klessinger and J. Michl, *Excited States and Photo-Chemistry of Organic Molecules*, Wiley, 1995.
- S. V. Bhat, B. A. Nagasampagi and M. Sivakumar, *Chemistry of Natural Products*, Narosa Publishing House, New Delhi, 2005.
- X.-T. Liang and W.-S. Fang, *Medicinal Chemistry of Bioactive Natural Products*, John Wiley & Sons, 2006.
- T. Hudlicky and J. W. Reed, *The Way of Synthesis*, Wiley-VCH, 2007.
- H. Osbon, Carbohydrates, Academic Press, 2003.
- I. L. Finar, *Organic Chemistry*, Volume 2: *Stereochemistry and The Chemistry Natural Products*, 5th edn, Pearson Education India, 1956.
- G. C. Howard and W. E. Brown, *Modern Protein Chemistry: Practical Aspects*, CRC Press, 2001.
- S. P. Bhutani, *Chemistry of Biomolecules*, CRC Press, 2010.

- O. Stone, Chemical Biology: *An Overview on Chemistry and Biology of the Biomolecules*, Foster Academics, 2015.
- T. Palmer, *Enzymes: Biochemistry, Biotechnology and Clinical Chemistry*, Horwood, 2001.
- T. D. H. Bugg, Introduction to Enzyme and Coenzyme Chemistry, 3rd edn, Wiley, 2012.

Physical Special

1. Connection Between Thermodynamics and Statistical Mechanics

Definition of Microstates and Macrostates. Boltzmann's definition of entropy. Formula for calculation of thermodynamic properties in terms of number of microstates. Determination of number of microstates for classical ideal gas. Connection among the properties of ideal gas, Gibbs paradox, Sackur-Tetrode equation.

2. Ensemble Method and its Application

Definition of ensemble. A priori probability. Gibbs postulate in Statistical mechanics. Ergodic hypothesis. Prescription for studying of thermodynamic systems based on ensemble method. Preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open). Determination of distribution function. Partition function. Calculation of thermodynamic properties in terms of partition function. Theory of Fluctuations. Calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc.

3. Boltzmann, Fermi-Dirac and Bose-Einstein Statistics

Canonical partition function for non-interacting distinguishable and non-identical particles. Boltzmann Statistics. Grand canonical partition function for non-interacting identical particles. Fermi-Dirac and Bose-Einstein statistics and their limiting behavior. Ideal monoatomic gas. The translational partition function. The electric and nuclear partition function. Thermodynamic function. Ideal diatomic gases. The rigid rotor-Harmonic oscillator approximation. The vibrational partition function. The rotational partition function of a heteronuclear molecule. The symmetry requirement of the total wave function of a homonuclear diatomic molecule. The rotational partition function of a homonuclear diatomic molecule. Thermodynamic function.

4. Classical and Quantum Statistics

The classical partition function. Phase space and the Liouville equation. Equipartition of energy. Ideal polyatomic gas. The vibrational and the rotational partition functions. Thermodynamic function. Hindered rotation. A weakly degenerate ideal Fermi-Dirac Gas. A strongly degenerate ideal Fermi-Dirac gas. A weakly degenerate ideal Bose-Einstein gas. A strongly degenerate ideal Bose-Einstein gas. An ideal gas of photons. The density matrix. The classical limit from the Quantum mechanical expression for Q.

Reference Books

- M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, John Wiley, New York, 1994.
- G. W. Castellan, *Physical Chemistry*, 3rd Edn, Narosa Publishing House, 1995.
- N. A. Gokcen and R. G. Reddy, *Thermodynamics*, Plenum Press, New York, 1996.
- G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall, India, 1997.
- P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.
- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.

Special Practical

CHEM 404C(PR): Marks: 50, Credit: 4

COMPUTER APPLICATION IN CHEMISTRY GENERAL

THEORY

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 retrival, 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, EBCIDIC), fixed and floating point arithmetic30.

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. 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).

4. 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.

5. Elements of C language

PRACTICAL

On-hand practical training with computers on selected chemical problems.

Reference Books

- 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.

CHEM 405E(PR): Marks: 50, Credit: 4

Inorganic Practical

1. Synthesis and Characterization of Inorganic Compounds Including Co-ordination Complexes, Assemblies

- Bi-, tri- and polydentate N, O donor ligands, oximes etc.
- Complexation and purification of complexes.
- Polyoxometalate.

- MOF and coordination polymer of commercially available ligands.
- Techniques for Growing of single crystals.
- Spectral, thermal, electrochemical and magnetic studies.

2. Synthetic Methods

Solution chemistry, solid state synthesis, sol-gel methods, multi-step synthesis, preparation of isomers, synthesis under inert atmosphere, electro-synthesis

3. Characterization

Quantitative and qualitative determination of ligand and metal, use of spectral techniques (UV - visible, IR, NMR, ESR, magnetic moment, analytical methods (conductance, TG, DSC, cyclic voltametry, coulometry)

4. Solvent Extraction

(a) Separation of Co and Ni using *n*-butyl alcohol and estimation of Co.
(b) Separation of Cu and Fe using *n*-butyl acetate and estimation of Cu.

5. Use of organic reagents for the estimation of various metal ions

(a) 8-Hydroxyquinoline ($A1^{3+}$, Ti^{3+}, Fe^{3+}).
(b) Pyrogallol (Bi^{3+}).
(c) Nitron (NO_3^-).
(d) Salicyladoxime (Ni^{2+} in presence of Cu^{2+}).
(e) Anthranilic acid (Cd^{2+}, Zn^{2+}, Co^{2+}).

Organic Practical

1. Organic Synthesis

Synthesis of model organic compounds involving typical multi-step reactions, isolation and purification of the intermediate and final products (as applicable) and their characterisation by recrystallisation, chromatographic separation (as applicable), determination of mp/bp (as the case may be), and spectral measurements. (Model Experiments/Reactions/Compounds).

A. Beckmann rearrangement: Benzanilide from benzene. (Benzene to Benzophenone to Benzophenone oxime to Benzanilide).

B. Synthesis of Heterocyclic compounds:

- Skraup synthesis: Quinoline from Aniline.
- Fischer indole synthesis: 2 Phenylindole from phenyl hydrazine.

C. Preparation involving chlorosulphonation.

D. Preparation involving Friedel-Crafts reaction.

E. Preparation involving diazo-coupling reaction.

F. Preparation involving Reimer-Tiemann reaction.

G. Coumarin ring synthesis.

H. Preparation of indane-1,3-dione.

At least four experiments to be carried out during Lab Session.

Physical Practical

1. To determine the effect of change of (i) temperature and (ii) concentration on the rate constant of hydrolysis of an ester.
2. To study the conductance behavior of strong and weak electrolytes.
3. To determine the cmc of SDS in Water and Water-Ethanol (1:1) mixture using conductometry.
4. To determine the hydrolysis constant of aniline hydrochloride by conductometry.
5. To study the titration of H_3PO_4 by NaOH using potentiometry.
6. To determine the concentration of different halides in a mixture by potentiometry.
7. To study the iodination of aniline at different pH.
8. To determine the rate constant of oxidation of iodide ions by hydrogen peroxide studying the kinetics as a clock reaction.
9. To determine the order and rate constant of the reaction between $HBrO_3$ and HI.