SYLLABUS (CBCS)

For

M.Sc. Course in Chemistry

To be effective from the session 2023-2024

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 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; the number of students in each major paper will be decided by the department on the basis of marks obtained in earlier semesters.

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 to 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) on any topic relevant to the subject/paper assigned by the concerned teacher.

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 Code	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
	CHEM 404C	Medicinal Chemistry	10	40	-	50	4
	Practical Paper						
	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; 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' remark to obtain 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 (except from 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, Credits - 24)

Theoretical Papers

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

1. Chemical Bonding - A Quantum Chemical Approach (15 Lectures)

The Born-Oppenheimer approximation, MO of homo- and heteronuclear diatomic molecules, MO of polynuclear AB_n type molecules, Koopmans' theorem, Walsh diagram, isolobal analogy, molecular term symbols, Huckel method of π-MO calculation in ethylene, allyl system etc.

2. Coordination Chemistry: Bonding, Stereochemistry and Structure (20 Lectures)

Fundamentals, Orgel diagram, Tanabe-Sugano diagram, molecular orbital, spectral properties, nephelauxetic effect, Racah parameter, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, lowering of symmetry, electronic, steric, Jahn-Teller and Renner-Teller effects on energy levels, conformation of chelator/congregator, structural equilibrium and implication, correlation of CFSE with spectroscopy.

3. Organometallic Chemistry I (20 Lectures)

Overview and striking difference, valence electron count, oxidation number and formal ligand charge; structure, bonding, spectral analysis and characterization of carbonyls, nitrosyls and related pi-acids, alkyl, alkene, alkyne, π-allyl, polyene and cyclopolyene compounds; metal carbenes and carbynes, hydride and dihydrogen complexes, isolobal analogy, Dewar-Chatt-Duncanson model, oxophilicity, agostic interaction; metal-carbon bonded compounds (σ-bonded), synthesis, reactivity, oxidative addition and reductive elimination reaction, insertion reactions.

4. Bioinorganic Chemistry (25 Lectures)

Metal ions in biology, O_2 - uptake proteins: haemoglobin, myoglobin, hemerythrin and hemocyanin, structure, function and model study, metal ion transport and storage proteins: ferritin, transferrin, ceruloplasmin; electron transport proteins: cytochromes, Fe-S proteins, blue copper proteins, biological fixation of nitrogen; urease, xanthine oxidase, sulphite oxidase, nitrate reductase; study of metalloprotein and metalloenzyme: superoxide dismutase, catalase, peroxidase, cytochrome P-450, cytochrome oxidase, carbonic anhydrase, carboxy peptidase, catechol oxidase, metallothionine; vitamin B_{12} and B_{12}-enzyme, photosynthesis, chlorophyll, PS-I, PS-II.

References:

- F. A. Cotton. Chemical Applications of Group Theory, 3rd Edn. John Wiley & Sons, New York, 1999.

- F. A. Cotton, G. Wilkinson, C. M. Murillo, M. Bochmann. Advanced Inorganic Chemistry, 6th Edn. John Wiley & Sons, New York, 1999.
- B. Douglas, D. McDaniel, J. Alexander. Concepts and Models of Inorganic Chemistry, 3rd Edn. John Wiley & Sons, New York, 2001.
- J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi. Inorganic Chemistry: Principles of Structures and Reactivity, 4th Edn. Pearson, New Delhi, 2006.
- H. E. White. Introduction to Atomic Spectra, McGraw-Hill Kogakusha Ltd, Tokyo, 1934.
- B. N. Figgis. Introduction to Ligand Field Theory, Interscience, New York, 1966.
- C. J. Ballhausen. Molecular Electronic Structure of Transition Metal Complexes, McGraw-Hill, London, 1979.
- R. McWeeney. Coulsons' Valence, 3rd Edn. Oxford University Press, Oxford, 1979.
- A. B. P. Lever. Inorganic Electronic Spectroscopy, Elsevier, New York, 1984.
- B. E. Douglas, C. A. Hollingsworth. Symmetry in Bonding and Spectra; an Introduction, Academic Press, New York, 1985.
- T. A. Albright, J. K. Burdett, M. H. Whangbo. Orbital Interactions in Chemistry, Wiley, New York, 1985.
- V. Heine. Group Theory in Quantum Mechanics: An introduction to its present usage, Dover publication, New York, 1991.
- P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong. Shriver & Atkins Inorganic Chemistry, 4th Edn. Oxford, 2006.
- P. Powell. Principles of Organometallic Chemistry, 2nd Edn. Chapman and Hall, London, 1988.
- J. D. Atwood. Inorganic and Organometallic Reaction Mechanisms, 2nd Edn. VCH, New York, 1997.
- R. H. Crabtree. The Organometallic Chemistry of the Transition Metals, 4th Edn. Wiley, New York, 2005.
- C. Elschenbroich. Organometallics, 3rd Edn. Wiley-VCH, Weinheim, 2006.
- R. A. Van Santen, M. Neurock. Molecular Heterogenous Catalysis, Wiley-VCH, Weinheim, 2006.
- G. O. Spessard, G. L. Miessler. Organometallic Chemistry, 2nd Edn. Oxford University Press, Oxford, 2010.
- J. F. Hartwig. Organotransition Metal Chemistry: from bonding to catalysis, University Science Books, Sausalito, CA, 2010.

- S. J. Lippard, J. M. Berg. Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, CA, 1993.
- W. Kaim, B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, Wiley, New York, 1994.
- I. Bertini, H. B. Gray, S. J. Lipperd, J. S. Valentine. Bioinorganic Chemistry, Viva books (P) Ltd. New Delhi, 1998.
- A. Das, G. N. Mukherjee. Elements of Bioinorganic Chemistry, 2nd Edn. U. N. Dhur & Sons, Kolkata, 2002.
- A. K. Das. Bioinorganic Chemistry, Books & allied (P) Ltd. Kolkata, 2007.
- E. Ochiai, Bioinorganic Chemistry: A Survey, Academic press, Elsevier, 2009.
- R. R. Crichten. Biological Inorganic Chemistry: A New Introduction to Molecular Structure, 2nd Edn. Elsevier, New York, 2012.
- R. M. Roat-Malone. Bioinorganic Chemistry: A Short Course, 2nd Edn. Wiley, New York, 2013.

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

1. Bonding in Organic Molecules & Structure-Reactivity Relationship (20 Lectures)

Qualitative MO treatment to acyclic and cyclic conjugated systems, Huckel treatment-applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene and benzene; concept of aromaticity in benzenoid and nonbenzenoid systems, 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 (20 Lectures)

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, 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 (20 Lectures)

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

4. Mass Spectroscopy (20 Lectures)

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, meta-stable peak, isotope, ion-molecule interaction and analysis of fragmentation patterns; calculation of MF from mass, introduction to GC-MS, LC-MS and MS-MS.

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

Reference Books:

- E. V. Anslyn, D. A. Dougherty. Modern Physical Organic Chemistry, University Science Books, 2006.
- S. Shaik, P. C. Hiberty. Valence Bond Theory, its History, Fundamentals and Applications: a Primer, Reviews in Computational Chemistry, Volume 20 (Eds. K. B. Lipkowitz, R. Larter, T. R. Cundari), John Wiley & Sons, Hoboken, NJ, USA, 2004.
- F. A. Caroll. Perspectives on Structure and Mechanism in Organic Chemistry, 2nd Edn. Wiley-VCH, 2011.
- E. L. Eliel, S. H. Wilson, L. N. Mander. Stereochemistry of Organic Compounds, John Wiley & Sons, 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, G. A. Morrison. Conformational Analysis, John Wiley & Sons, 1967.
- J. Eames, J. Peach. Stereochemistry at a Glance, Blackwell Science, 2003.
- K. Mislow, 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, 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, J. March. March's Advanced Organic Chemistry (Reactions, Mechanisms and Structure), 5th Edn. John Wiley & Sons, 2001.
- L. N. Ferguson. The Modern Structural Theory of Organic Chemistry, Prentice-Hall of India Pvt. Ltd., New Delhi, 1963.
- R. H. Grubbs, D. J. O'leary. Handbook of Metathesis - Volume 1 & 2, Wiley-VCH, 2015.
- D. L. Pavia, G. M. Lampman, G. S. Kriz. Introduction to Spectroscopy, 3rd Edn. Harcourt, 2001.
- R. M. Silverstein, G. C. Bassler, T. C. Morrill. Spectroscopic Identification of Organic Compounds, 5th Edn. John Wiley & Sons, 1991.
- D. H. Williams, 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, D. H. Williams. Interpretation of Mass Spectra of Organic Compounds. Holden-Day Inc., 1965.
- J. S. Splitter, F. Turećek. Applications of Mass Spectrometry to Organic Stereochemistry, Wiley-VCH, 1994.
- Atta-ur-Rahman, Md. Iqbal Choudhary. Solving Problems with NMR Spectroscopy, Academic press, 1996.
- N. S. Bhacca, D. H. Williams. Applications of NMR Spectroscopy in Organic Chemistry, Holden-Day Inc., 1964.
- L. M. Jackman, 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, J. B. Macmillan. Problems in Organic Structure Determination: a Practical Approach to NMR Spectroscopy, CRC press, Taylor & Francis group, 2016.
- Y. R. Sharma. Elementary Organic Spectroscopy (Principles and Chemical Applications) S. Chand & Company ltd., New Delhi, 5th Edn. 2013.

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

1. Quantum Mechanics I **(16 Lectures)**

Introduction, properties of sets of wave functions; operators - linear and nonlinear operators, Laplacian operator, Hermitian operators and their properties, eigen-functions and eigenvalues of an operator; eigenvalue equation, eigen-functions of commuting operators; expectation values;

time-dependent Schrödinger equation of motion, conservative systems and time independent Schrödinger equation; particle in a one and three-dimensional boxes with infinite potential walls, important features, Bohr's correspondence principle.

2. Symmetry & Group Theory I (16 Lectures)

Introduction, 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.

3. Electrochemistry (12 Lectures)

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.

4. Biophysical Chemistry (18 Lectures)

Introduction, adsorption of solids, micelles, reverse micelles, microemulsion, thermodynamics of micellization, hydrophobic hydration, interaction; stabilization and denaturation of protein, transport of ions, ion channels, configuration and conformation of biological macromolecules, membrane structure; applications of spectroscopic techniques: UV-Vis, CD, fluorescence, separation techniques : gel electrophoresis; macromolecule ligand binding and co-operativity.

5. Chemical Kinetics I (18 Lectures)

Introduction, theories of reaction rates: applications to uni-, bi- and ter-molecular 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 equations; fast reactions: flow process and relaxation techniques.

Reference Books:

- L. Pauling, E. B. Wilson. Introduction to Quantum Mechanics, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter, 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, New Delhi, 1989.
- F. L. Pilar. Elementary Quantum Chemistry, Tata McGraw-Hill, New Delhi, 1990.
- D. A. McQuarrie. Quantum Chemistry, Viva books (P) Ltd. New Delhi, 2003.
- S. C. Rakshit. Molecular Symmetry Group and Chemistry, The New Book Stall, Kolkata, 1988.
- F. A. Cotton. Chemical Applications of Group Theory, 3rd Edn. John Wiley & Sons. New York, 1999.
- D. M. Bishop. Group Theory and Chemistry, Oxford University Press, 1993.
- J. Vincent. Molecular Symmetry and Group Theory, John Wiley & Sons. New York, 1998.
- S. Glasstone. An Introduction to Electrochemistry, D. Van Nostrand Company, 1962.
- J. O'M. Bockris, A. K. N. Reddy. Modern Electrochemistry, Volume I, Plenum Press, New York, 1970.
- J. Albery. Electrode Kinetics, Oxford Chemistry Series, Clarendron Press, Oxford, 1975.
- G. W. Castellan. Physical Chemistry, 3rd Edn. Narosa Publishing House, New Delhi, 1995.
- R. A. Alberty, R. J. Silbey. Physical Chemistry, 1st Edn. John Wiley & Sons. New York, 1995.
- R. S. Berry, S. A. Rice, J. Ross. Physical Chemistry, Oxford University Press, London, 1970.
- K. V. Van Holde, W. C. Johnson, P. S. Ho. Principles of Physical Biochemistry, Prentice Hall, 1998.
- D. L. Nelson, M. Cox. Lehninger Principles of Biochemistry, 8th Edn. Macmillan Learning, 2017.
- C. Tanford. Physical Chemistry of Macromolecules, John Wiley & Sons. New York, 1961.
- P. J. Flory. Principles of Polymer Chemistry, Cornell University Press, Ithaca & London, 1995.
- K. J. Laidler. Reaction Kinetics, Volume I & II, Pergamon Press, London, 1970.
- K. J. Laidler. Chemical Kinetics, Tata McGraw-Hill Publishing Company Ltd. New Delhi, 1988.
- M. R. Wright. Fundamental Chemical Kinetics, Horwood Publishing, 1999.

Practical Papers

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

1. Inorganic qualitative analysis of rare earth elements.

2. Synthesis and characterization of inorganic and co-ordination compounds: selected simple salts, double salts and co-ordination compounds with some commercially available inorganic and organic ligands.

Reference Books:

- G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney. Vogel's Textbook of Quantitative Chemical Analysis. 5th Edn. John Wiley & Sons, New York, 1989.
- G. N. Mukherjee. Advanced Experiments in Inorganic Chemistry, 2nd Edn. U. N. Dhur & Sons Pvt. Ltd. 2018.
- Dr. L. R. Sharma. Practical Inorganic Chemistry, Evincepub Publishing, 2021.

CHEM 105C(PR): Organic Chemistry Practical **Marks: 50, Credits: 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-, alcoholic -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

1. Oxidation of benzylic carbon by prior protection of $-NH_2$ group in the nucleus followed by deprotection: 4-aminobenzoicacid from 4-aminotoluene.

2. Preparation of imide followed by Hofmann degradation: anthranilic acid from phthalic anhydride.

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

4. Oxidation of α-hydroxyketone to diketone followed by rearrangement benzilic acid from benzoin.

5. 1,4-dihydropyridine ring generation: ethyl acetoacetate to 2,6-dimethyl-3,5-dicarbethoxy-1,4-dihydropyridine.

6. Partial reduction of aromatic dinitro compound: m-dinitrobenzene to m-nitroaniline.

7. Benzoylation of amino group in presence of carboxylic acid group: glycine to hippuric acid.

8. Reduction of a hydroxycarboxylic acid with HI and red P: benzilic acid to diphenylacetic acid.

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

Reference Books:

- B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell. Vogel's Textbook of Practical Organic Chemistry, 5th Edn. John Wiley & Sons. New York, 1989.
- A. I. Vogel. A Textbook of Practical Organic Chemistry, 3rd Edn. Longman Group Ltd. London, 1956.
- R. C. Bhattacharyya. A Manual of Practical Chemistry, 11th Edn. Studies Book Sellers & Publishers, Calcutta, 1992.
- Roberts, Gilbert, Rodewaid, Wingrove. An Introduction to Experimental Organic Chemistry, 3rd Edn. Holt, Rinehart & Winston Publishers, New York, 1969.
- H. T, Clarke. Handbook of Organic Analysis, 4th Edn. Hodder & Stoughton Educational, London, 1926.
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- V. K. Ahluwalia, R. Aggarwal. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press, 2001.
- E. Stahl. Thin Layer Chromatography, 2nd Edn. Springer, 1969.
- R. M. Silverstein. Spectrometric Identification of Organic Compounds, 6th Edn. John Wiley & Sons, New York, 1997.

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

Theoretical Papers

CHEM 201C: Inorganic Chemistry **Marks: 50, Credits: 4**

1. Thermoanalytical Methods **(14 Lectures)**

Different methods of analysis: TGA, DTA, DSC; thermogram, thermal stability of covalent and noncovalent bonds, thermal degradation, single crystal phase transformation, thermo-chemiluminescence, thermometric titration, solid state reaction kinetics.

2. Electroanalytical Methods **(16 Lectures)**

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

3. Nuclear Chemistry **(18 Lectures)**

Introduction to nuclear stability, formulation of semi-empirical binding energy equation, mass parabola, application of binding energy equation; nuclear reactions, Q value and cross section of nuclear reaction, liquid drop model, Fermi gas model, magic numbers and its derivation from nuclear potential well, nuclear fission and fusion; nuclear reactors and particle accelerators; interaction of radiation with matter, radio-analytical techniques and activation analysis.

4. Environmental Chemistry **(16 Lectures)**

Organic and inorganic pollutants, pesticides and their chemical speciation; eutrophication, waste water treatment - primary, secondary and tertiary treatment, nuclear waste; nuclear accidents, control of air pollution: different methods - gravitational setting chamber, cyclone separators, electrostatic precipitator; various sources of soil pollution; solid waste management; noise pollution: classification, hazards; microwave and ultrasound assisted green synthesis.

5. Molecular Magnetism I **(16 Lectures)**

Different magnetic materials, use of Pascal's constants in structure determination, van Vleck equation and its application, Curie-Weiss law and its implication, Lande interval rule, microstates, multiplet, multiplet width, hole formalism, zero-field splitting, spin-orbit coupling, quenching of orbital contribution, crystal field, diagram, high spin/low spin equilibrium, Fermi contact and pseudo-contact shifts, chemical shift reagent.

Reference Books:

- C. Duval. Inorganic Thermogravimetric Analysis, Elsevier Publishing Co, New York, 1963.

- W. W. Wendlandt. Thermal Methods of Analysis, Interscience Publishers, New York, 1964.
- R. C. McKenzie (Ed). Differential Thermal Analysis, Academic Press, New York, 1970.
- D. Dollimore. General Review on Thermal Analysis, Analytical Chemistry, 1994, 66, 17R.
- S. M. Khopkar. Basic Concepts of Analytical Chemistry, Wiley Eastern Ltd. New Delhi, 1998.
- D. R. Crow. Polarography of Metal Complexes, Academic Press, London, 1979.
- A. J. Bard, L. F. Faulkner. Electrochemical Methods - Fundamentals and Applications, 2nd Edn. Wiley, New York, 1998.
- C. G. Zoski (Ed). Handbook of Electrochemistry, Elsevier, New York, 2007.
- H. J. Arnikar, Essentials of Nuclear Chemistry, 4th Edn. New Age International (P) Ltd. New Delhi, 2001.
- R. D. Evans. The Atomic Nucleus, McGraw-Hill, New York, 1979.
- B. Harvey. Introduction to Nuclear Physics and Chemistry, Prentice Hall, 1965.
- S. Glasstone. Source Book of Atomic Energy, East-West Press Pvt. Ltd. New Delhi, 1967.
- D. F. S. Natusch, P. K. Hopke. Analytical Aspects of Environmental Chemistry, John Wiley & Sons, New York, 1983.
- R. M. Harrison (Ed). Pollution: Causes, Effects and Control, Royal Society of Chemistry, Great Britain, 1990.
- J. E. Fergusson. The Heavy Elements: Chemistry, Environmental Impact and Health Effects, Pergamon Press, Oxford, 1990.
- S. E. Manahan, Environmental Chemistry, Lewis Publishers, Boston, 1991.
- A. K. De. Environmental Chemistry, 4th Edn. New Age International (P) Ltd. New Delhi, 2000.
- J. S. Miller, M. Drillon (Ed). Magnetism: Molecules to Materials V; Molecule-Based Magnets, Wiley-VCH, Weinheim, 2005.
- F. E. Mabbs, D. J. Machin. Magnetism and Transition Metal Complexes, Dover Publications, New York, 2008.
- R. Winpenny (Ed). Single Molecule Magnets and related Phenomenon, Structure and Bonding Series, Volume 122, Springer, Berlin, 2010.
- B. D. Cullity, C. D. Graham, Introduction to Magnetic Materials, 2nd Edn. John Wiley & Sons, New York, 2011.
- D. Gatteschi, R. Sessoli, J. Villain. Molecular Nanomagnets, Oxford University Press, Oxford, 2006.

- R. Hilzinger, W. Rodewald. Magnetic Materials, Wiley, New York, 2013.
- P. M. Lathi (Ed). Magnetic Properties of Organic Materials, Marcel Dekker, New York, 1999.

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

1. Heterocyclic Chemistry I **(15 Lectures)**

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

2. Organic Name Reaction and Reagents **(30 Lectures)**

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

3. Pericyclic Reactions **(20 Lectures)**

The Woodward-Hoffmann selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, cheleotropic reactions and group transfer reaction, rationalization based on frontier MO 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+2Π), (4Π+2Π), (4Π+4Π), (2Π+2Π+2Π)] and metal catalysed cycloaddition reactions.

4. Asymmetric Synthesis I **(15 Lectures)**

Introduction to asymmetric synthesis, preliminary idea about different methods of asymmetric synthesis with special reference to the chiral pool strategy, asymmetric Diels-Alder reaction, Heck reaction and aza-Baylis-Hillman reaction, enantioselective organocatalysis, biocatalysis.

Reference Books:

- T. L. Gilchrist, R. C. Storr. Organic Reactions and Orbital Symmetry, 2nd Edn. Cambridge University Press, 1979.
- N. J. Turro. Modern Molecular Photochemistry, The Benjamin Cummings Publishing, 1978.

- S. Sankararaman. Pericyclic Reactions - A Textbook, Wiley-VCH Verlag, 2005.
- R. E. Gawley, J. Aube. Principles of Asymmetric Synthesis, Elsevier, 1996.
- M. Gruttadauria, 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, 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, K. Mills. Heterocyclic Chemistry, Blackwell Science Publication, 2000.
- R. K. Bansal. Heterocyclic Chemistry: Synthesis, Reactions and Mechanisms, Wiley Eastern Ltd. New Delhi, 1999.
- T. L. Gilchrist. Heterocyclic Chemistry, Pearson Education, 2008.
- T. Eicher, S. Hauptmann, 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 Synthesis based on Name Reactions, 3rd Edn. Elsevier, 2012.
- L. Kürti, B. Czakó. Strategic Applications of Name 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, J. March. March's Advanced Organic Chemistry (Reactions, Mechanisms and Structure), 5th Edn. John Wiley & Sons, 2001.
- R. Bruckner. Advanced Organic Chemistry (Reaction Mechanisms), Harcourt Academic Press, 2002.
- J. Clayden, N. Greeves, S. Warren, P. Wothers. Organic Chemistry, Oxford University Press, 2001.
- F. A. Carry, R. J. Sundberg. Advanced Organic Chemistry, 5th Edn. Springer, 2007.
- L. G. Wade, Jr. M. S. Singh. Organic Chemistry, 6th Edn. Pearson Education, 2008.
- T. G. Graham, 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, S. K. Bhattacharjee. Organic Chemistry, 7th Edn. Pearson Education, 2013.
- W. Carruthers, I. Coldham. Modern Methods of Organic Synthesis, Cambridge University Press, 4th Edn. 2012.

CHEM 203C: Physical Chemistry **Marks: 50, Credits: 4**

1. Quantum Mechanics II **(14 Lectures)**

Free particle in one dimension; particle in one dimensional box with finite potential walls (or particle in a rectangular well), step potential and tunneling; solution of Schrodinger equation of a Harmonic oscillator using the operator method; selection rules for Harmonic oscillator; rigid rotator; elementary discussion of the H-atom solution; Heisenberg's uncertainty principle.

2. Photo-excited Processes **(16 Lectures)**

Introduction, Jablonski diagram, photoexcitation, fluorescence, phosphorescence, photosensitization, delayed fluorescence: E- and P-type, quantum yield and its determination, fluorescence quenching: static and dynamic, application of Stern-Volmer equation/plot (linear and non-linear); absorption, emission and excitation spectra - mirror symmetry, excited state processes, Marcus theory, solvent effect in spectroscopy, solvation dynamics, sensing of biologically relevant cations, anions and neutral molecules, chemosensors.

3. Nanotechnology: Principles and Applications **(16 Lectures)**

Introduction, fundamental principles of nanoparticles (0D, 1D, 2D and 3D) and their physical, optical, electronic, magnetic properties; metallic and semiconducting nanoparticles; density of states, some special nanomaterials - quantum wire, thin film, fullerenes, carbon nanotubes and nanodiamonds; nanolithography; material characterization techniques: transmission electron microscopy (TEM), scanning electron microscope (SEM) and atomic force microscopy (AFM); applications of nanotechnology.

4. Thermodynamics and Statistical Mechanics **(16 Lectures)**

Introduction, Legendre transformation with applications; Maxwell-Boltzmann distribution with degeneracy (distinguishable and indistinguishable particles), partition function and its properties, interpretation of thermodynamic laws, thermodynamic functions in terms of partition functions, molecular partition functions (translational, rotational, vibrational and electronic) for ideal gas, Sackur-Tetrode equation, calculation of thermodynamic functions for mono- and diatomic gases, equipartition principle, equilibrium constant in terms of partition functions.

5. Crystal Structure **(18 Lectures)**

Introduction, 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, Brillouin zones and Fermi level in lattice, concept of particle-hole, band theory, 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: single crystal and powder XRD.

Reference Books:

- L. Pauling, E. B. Wilson. Introduction to Quantum Mechanics, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter, 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, New Delhi, 1989.
- F. L. Pilar. Elementary Quantum Chemistry, Tata McGraw-Hill, New Delhi, 1990.
- D. A. McQuarrie. Quantum Chemistry, Viva Books Pvt Ltd, New Delhi, 2003.
- J. R. Lakowicz. Principles of Fluorescence Spectroscopy, 3rd Edn. Springer, 2010.
- N. J. Turro. Modern Molecular Photochemistry, The Benjamin Cummings Publishing, 1978.
- B. Valeur, M. N. Berberan-Santos. Molecular Fluorescence: Principles and Applications, John Wiley & Sons, New York 2012.
- K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International (P) ltd, India, 2007.
- C. Bréchignac, B. P. Houdy, M. Lahmani. Nanomaterials and Nanochemistry, Springer, London, 2006.
- C. N. R. Rao, A. Muller, A. K. Cheetam. The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Wiley-VCH verlog, Germany, 2005.
- G. Cao. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press, London, 2004.
- R. W. Kelshell, I. W. Hameley, M. Geoghegan. Nanoscale Science and Technology, John Wiley & Sons, England, 2005.
- C. P. Poole, F. J. Owens. Introduction to Nanotechnology, Wiley Interscience, 2003.

- T. Pradeep. A Textbook of Nanoscience and Nanotechnology, Tata McGraw-Hill India, 2012.
- P. Diwan, A. Bharadwaj. The Nanoscope: Encyclopedia of Nanoscience and Nanotechnology. Pentagon Press, 2005.
- N. Levine. Physical Chemistry, Tata McGraw-Hill, New Delhi, 1978.
- K. Denbigh. Principles of Chemical Equilibrium, Cambridge University Press, Cambridge, 1981.
- M. Klotz, R. M. Rosenberg. Chemical Thermodynamics, John Wiley & Sons, New York, 1994.
- G. W. Castellan. Physical Chemistry, 3rd Edn. Narosa Publishing House, 1995.
- N. A. Gokcen, R. G. Reddy. Thermodynamics, Plenum Press, New York, 1996.
- P. W. Atkins. Physical Chemistry, Oxford University Press, Oxford, 1998.
- R. S. Berry, S. A. Rice, J. Ross. Physical Chemistry, Oxford University Press, Oxford, 2000.
- G. D. Mahan. Many Particle Physics, Kluer Academy, Plenum Publisher, 2000.
- C. 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, R. A. Palmer. Structure Determination by X-ray Crystallography, 3rd Edn. Plenum Press.
- X. Clegg. Crystal Structure Determination, Oxford University Press, Oxford, 2005.

Practical Papers

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

1. Computer application in chemistry-Exposure to available standard application packages like: chemdraw, generation of graphs using Origin, data sheet creation, tables using excel programme etc.
2. Experiments on quantitative estimation: analysis of selected ores, minerals and alloys.
   (a) Analysis of brass (Cu and Zn) by iodometry and complexometry.
   (b) Analysis of dolomite (Ca, Mg, Fe) by complexometry
   (c) Analysis of bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2) by gravimetry (SiO_2), complexometry (Al^{3+}), redox titration using Jones reductor (Fe^{3+} and Ti^{4+}), Spectrophotometric estimation of Fe^{3+}, Ti^{4+}.

Reference Books:

- G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney. Vogel's Textbook of Quantitative Chemical Analysis. 5th Edn. John Wiley & Sons, New York, 1989.
- G. N. Mukherjee. Advanced Experiments in Inorganic Chemistry, 2nd Edn. U. N. Dhur & Sons Pvt. Ltd. 2018.
- Dr. L. R. Sharma. Practical Inorganic Chemistry, Evincepub Publishing, 2021.

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

- To determine the rate constant of acid catalyzed hydrolysis of an ester in a micellar media.
- To verify Ostwald dilution law and determine the K_a of a weak acid.
- To determine the rate constant and salt effect on the rate constant of the reaction between $K_2S_2O_8$ and KI.
- To determine the composition of a mixture of acetic acid, sodium acetate and ammonium acetate by conductometry.
- To investigate the kinetics of inversion of canesugar by polarimeter.
- To determine the composition of metal-ligand complex by Job's method.

Reference Books:

- B. Viswanathan, P. S. Raghavan. Practical Physical Chemistry, Viva Books, 2009.
- J. Mendham. Vogel's Quantitative Chemical Analysis, 6th Edn. Pearson Education, 2009.
- D. C. Harris. Quantitative Chemical Analysis, 6th Edn. W. H. Freeman, 2007.
- S. R. Palit, S. K. De. Practical Physical Chemistry, Science Book Agency.
- University Hand Book of Undergraduate Chemistry Experiments, edited by G. N. Mukherjee. University of Calcutta.
- B. P. Levitt. Findlay's Practical Physical Chemistry, 9th Edn. Longman Group Ltd. 1973.
- J. N. Gurtu, R. Kapoor. Advanced Experimental Chemistry, S. Chand & Co. Ltd.

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

Theoretical Papers

CHEM 301C: Inorganic Chemistry **Marks: 50, Credits: 4**

1. Chemistry of Inner Transition Elements **(18 Lectures)**

Comparison of characteristics of inner transition and transition metals; source, extraction and applications; 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. Silicates and Aluminosilicates **(12 Lectures)**

Classification; structure, properties and applications of silicates and aluminosilicates; characterization of clays and zeolites; zeolitic structures; structure area, surface activity, pore size, application of clays and zeolites, MOFs with zeolitic structure, reticular syntheses.

3. Inorganic Photochemistry **(20 Lectures)**

Introduction to inorganic photochemistry; photo-physical and photo-chemical processes; Excitation modes in transition metal complexes; fate of photo-excited species; fluorescence and phosphorescence applied to inorganic systems; intra-molecular energy transfer; vibrational relaxation, internal conversion and intersystem crossing, quantum yield, decay fluorescence; fluorescence quenching; Stern-Volmer equation; photochemical process: photo substitution and photo electron 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 co-ordination compounds - synthesis and catalysis, solar energy conversion and storage.

4. Inorganic Chains, Rings, Cages and Clusters **(15 Lectures)**

Phosphazenes; homo- and heterocyclic inorganic ring systems; polymorphism of C, P and S; structure and bonding in higher boranes and borohydrides - Lipscomb's topological models; Wade's rules; polyhedral skeletal electron pair theory (PSEPT); carboranes and metallo-carboranes; metal clusters; giant clusters and synthesis methodology; 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.

5. Inorganic Reaction Mechanism I **(15 Lectures)**

Energy profile diagrams 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 substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes; aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution.

Reference Books:

- J. D. Lee. Concise Inorganic Chemistry, ELBS, 1991.
- B. E. Douglas, D. H. McDaniel. Concepts & Models of Inorganic Chemistry, Oxford, 1970.
- M. C. Dey, J. Selbin. Theoretical Inorganic Chemistry, ACS Publications, 1962.
- N. N. Greenwood, A. Earnshaw. Chemistry of the Elements, Butterworth-Heinemann, 1997.
- P. Atkins. Shriver and Atkins Inorganic Chemistry, 5th Edn. Oxford University Press, 2010.
- F. A. Cotton, G. Wilkinson, P. L. Gaus. Basic Inorganic Chemistry, 3rd Edn. Wiley India.
- J. E. Huheey, E. A. Keiter, R. L. Keiter. Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edn, Harper Collins 1993, Pearson, 2006.
- B. Douglas, D. McDaniel, J. Alexander. Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
- G. L. Miessler, D. A. Tarr. Inorganic Chemistry, 3rd Edn, Pearson, New Delhi, 2009.
- M. J. Malin. The Chemistry and Mechanism of Art Materials, 1st Edn, CRC Press, 2021.
- W. A. Harrison. Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds, Dover Publications, New York, 1989.
- K. J. Klabunde. Free Atoms, Clusters and Nanoscale Particles, Academic Press, New York, 1994.
- D. M. P. Mingos, D. J. Wales. Introduction to Cluster Chemistry, Prentice Hall, New York, 1990.
- D. F. Shriver, H. D. Kaesz, R. D. Adams. The Chemistry of Metal Cluster Complexes, VCH, New York, 1990.

- W. Adamson, P. D. Fleischauer. Concept of Inorganic Photochemistry, Wiley, New York, 1975.
- G. L. Geoffroy, M. S. Wrighton. Organometallic Photochemistry, Academic Press, New York, 1970.
- R. Hollebone, C. H. Langford, N. Serpone. Inorganic Photochemistry, Coordination Chemistry Review, 1981, 39, 181.
- F. Basolo, R. G. Pearson. Mechanism of Inorganic Reactions, 2nd Edn, Wiley, New York, 1967.
- D. Katakis, G. Gordon. Mechanisms of Inorganic Reactions, John Wiley & Sons, New York, 1987.

CHEM 302C: Organic Chemistry **Marks: 50, Credits: 4**

1. Synthetic Methodology and Advance Organic Synthesis (25 Lectures)

Organoboron compounds: Hydrocarbon reaction and its synthetic application; applications of organoboranes; Isomerisation of organoboranes; formation of carbon-carbon bonds; formation of aldehydes, ketones, trialkylcarbinols; reactions of alkenylboranes and trialkyl alkynyl borates; free radical reactions of organoborane.

Organophosphorus compounds: Chemistry of organophosphorus compounds; phosphorous ylids; chiral phosphines.

Organosulphur compounds: Chemistry of organosulphur compounds; sulphur stabilized 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 acyl silanes; Brook rearrangement; silicon Baeyer Villiger rearrangement.

2. Green Chemistry and Nanoscience (15 Lectures)

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; tools of green chemistry; real world cases of practicing green chemistry.

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 **(20 Lectures)**

Alkaloids: 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; biogenesis of alkaloids and terpenoids.

4. Organometallic Chemistry of Transition Elements **(20 Lectures)**

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, Negishi, Sonogashira, Kumada, Hiyama, Ziegler-Natta reaction; olefin metathesis; Tebbe's reagent, Pauson-Khand reactions; Volhsrdt co-trimerisation, functional organometallic compounds; use of non-transition metals - tin and zinc in organic synthesis.

Reference Books:

- M. Schlosser, K. Smith. Organoboron Chemistry, Wiley-VCH, 2013.
- M. G. Davidson, K. Wade, T. B. Marder, A. K. Hughes. Contemporary Boron Chemistry, Royal Society of Chemistry, 2000.
- B. Marciniec. Progress in Organosilicon Chemistry, Taylor & Francis, 1995.
- N. Auner, J. Weis. Organosilicon Chemistry 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, J. C. Tebby. Organophosphorous Chemistry, RSC Book Series.
- P. G. M. Wuts, T. W. Greene. Greene's Protective Groups in Organic Synthesis, 4th Edn, Wiley-VCH, 2006.
- E. J. Corey, X.-M. Chelg. The Logic of Organic Synthesis, John Wiley & Sons, 1995.
- P. T. Anastas, J. C. Warner. Green Chemistry: Theory and Practice, Oxford University Press, 2000.
- P. T. Anastas. Handbook of Green Chemistry, Wiley-VCH Book Series.
- J. H. Clark. RSC Green Chemistry, Royal Society of Chemistry Book Series.
- V. K. Ahluwalia, K. Kidwai. New Trends in Green Chemistry, Springer, 2004.

- R. A. Sheldon, I. Arends, U. Hanefeld. Green Chemistry and Catalysis, Wiley-VCH, 2007.
- A. K. Kruthiventi, 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, 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, G. L. Miessler. Organometallic Chemistry, Oxford University Press, 2010.
- D. Gupta. Basic Organometallic Chemistry: Concepts, Synthesis and Applications, Universities Press, 2011.
- D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.

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

1. Group Theory II **(20 Lectures)**

The Great Orthogonality Theorem (GOT) - 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 vibrational mode, selection rules for Infrared and Raman spectra, crystal field splitting.

2. Principle of Lasers and its Applications **(15 Lectures)**

Introduction, non-linear optical processes, stimulated emission of radiation, principles of laser action, two level transition (absorption, induced and stimulated emission), population inversion (two/three/four level systems), cavity modes, Q-switching, mode locking, various types of lasers: Ruby laser, Nd-YAG laser, diode laser, He-Ne laser, N_2 laser, Ar laser, excimer and exciplex laser, dye laser, applications of lasers.

3. Macromolecules (10 Lectures)

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. Chemical Kinetics II (15 Lectures)

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

5. Thermodynamics of Irreversible Processes (20 Lectures)

Limitations of classical (equilibrium) thermodynamics, entropy production in some simple irreversible processes, the concept of forces and fluxes, linear phenomenological relations; Onsager reciprocity relation - derivation from fluctuation theory; Curie-Prigogine principle - statement and proof using one scalar and one vector force, illustrations; Saxen's relations in connection with electrokinetic phenomena and their proof using Onsager reciprocity relations, stationary states: variation of entropy production with time, Prigogine's criterion for establishment of stationary state, applicability of Le Chateliar's principle on stationary states.

Reference Books:

- S. C. Rakshit. Molecular Symmetry Group and Chemistry, The New Book Stall, Kolkata, 1988.
- F. A. Cotton. Chemical Applications of Group Theory, 3rd Edn. John Wiley & Sons. New York, 1999.
- D. M. Bishop. Group Theory and Chemistry, Oxford University Press, 1993.
- J. Vincent. Molecular Symmetry and Group Theory, John Wiley & Sons. New York, 1998.
- W. Demtröder. Laser Spectroscopy, Springer Berlin, Heidelberg, 2008.
- P. Walsh. Lasers and Their Applications, EDTECH, 2018.
- K. Thyagarajan, A. Ghatak. Lasers: Theory and Applications, Springer US, 1981.
- P. J. Flory. Principles of Polymer Chemistry, Cornell University Press, New York, 1953.
- M. M. Coleman, P. C. Painter. Fundamentals of Polymer Science - An Introductory Text, 2nd Edn. CRC Press, 1997.

- W. Billmeyer. Text Book of Polymer Science, 2nd Edn, Wiley-Interscience, New York, 1971.
- K. J. Laidler, Reaction Kinetics, Volume I and II, Pergamon Press, London, 1970.
- K. J. Laidler, Chemical Kinetics, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.
- M. R. Wright, Fundamental Chemical Kinetics, Horwood Publishing, 1999.
- B. H. Lavanda. Thermodynamics of Irreversible Processes, Macmillan Education UK, 1978.
- I. Prigogine. Introduction to Thermodynamics of Irreversible Processes, Interscience Publishers, 1955.
- M. Klotz, R. M. Rosenberg. Chemical Thermodynamics, John Wiley & Sons, New York, 1994.
- N. A. Gokcen, R. G. Reddy. Thermodynamics, Plenum press, New York, 1996.

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

1. Chemical 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. Column chromatographic separation of binary mixture of organic compounds and choice of eluent.

(At least 6 samples are to be separated during the lab session).

Reference Books:

- B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell. Vogel's Textbook of Practical Organic Chemistry, 5th Edn. John Wiley & Sons. New York, 1989.
- A. I. Vogel. A Textbook of Practical Organic Chemistry, 3rd Edn. Longman group ltd. London, 1956.
- R. C. Bhattacharyya. A Manual of Practical Chemistry, 11th Edn. Studies book sellers & publishers, Calcutta, 1992.
- Roberts, Gilbert, Rodewaid, Wingrove. An Introduction to Experimental Organic Chemistry, 3rd Edn. Holt, Rinehart & Winston publishers, New York, 1969.
- H. T, Clarke. Handbook of Organic Analysis, 4th Edn. Hodder & Stoughton Educational, London, 1926.
- H. Middleton. Systematic Qualitative Organic Analysis, 2nd Edn. Hodder & Stoughton educational, London, 1943.

- V. K. Ahluwalia, R. Aggarwal. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press, 2001.
- E. Stahl. Thin Layer Chromatography, 2nd Edn. Springer, 1969.
- R. M. Silverstein. Spectrometric Identification of Organic Compounds, 6th Edn. John Wiley & Sons, New York, 1997.

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

- To determine the concentrations of a strong and a weak acid in a given mixture by potentiometry.
- To determine the formal potential of Fe(III)/ Fe(II) couple by potentiometry.
- To determine the dissociation constant of Phenolphthalein indicator by spectrophotometry.
- To study the kinetics of alkaline hydrolysis of crystal violet by spectrophotometry.
- Determination of pKa of a weak monobasic and pK_1 & pK_2 of a dibasic acid pH metrically.
- Determination of E_0 value of Ag^+/Ag electrode potentiometrically.

Reference Books:

- B. Viswanathan, P. S. Raghavan. Practical Physical Chemistry, Viva Books, 2009.
- J. Mendham. Vogel's Quantitative Chemical Analysis, 6th Edn. Pearson Education, 2009.
- D. C. Harris. Quantitative Chemical Analysis, 6th Edn. W. H. Freeman, 2007.
- S. R. Palit, S. K. De. Practical Physical Chemistry, Science Book Agency.
- University Hand Book of Undergraduate Chemistry Experiments, edited by G. N. Mukherjee. University of Calcutta.
- B. P. Levitt. Findlay's Practical Physical Chemistry, 9th Edn. Longman Group Ltd. 1973.
- J. N. Gurtu, R. Kapoor. Advanced Experimental Chemistry, S. Chand & Co. Ltd.

CHEM 305 EID **Marks: 50, Credits: 4**

1. Structure and Properties of Organic Molecules **(35 Lectures)**

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; delocalized bonds, inductive effect, resonance, steric inhibition of resonance, hyperconjugation, tautomerism, aromaticity, Huckel's rules, aromatic, nonaromatic and antiaromatic compounds, non-benzenoid aromatic compounds; formation, structure, stability and reactions of classical and non-classical carbocations, carbanions, free radicals, arynes, ylides, carbenes and nitrenes.

2. Atomic Structure **(25 Lectures)**

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 **(20 Lectures)**

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, Volume I, 6th Edn, Addison Wesley Longmann, London, 1998.
- I. L. Finar. Organic Chemistry, Volume 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, 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, P. Wothers. Organic Chemistry, Oxford University Press, 2001.
- F. A. Carry, R. J. Sundberg. Advanced Organic Chemistry - Part-A and B, 5th Edn, Springer, 2007.
- L. G. Wade. Jr., M. S. Singh. Organic Chemistry, 6th Edn, Pearson Education, 2008.
- J. Moody. Reactive Intermediates, Oxford University Press, 1992.

- R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee. Organic Chemistry, 7th Edn, Pearson Education, 2013.
- J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi. Inorganic Chemistry: Principles of Structures and Reactivity, 4th Edn, Pearson, New Delhi, 2006.
- F. A. Cotton, G. Wilkinson, C. M. Murillo, M. Bochmann. Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons Inc. New York, 1999.
- P. Atkins, T. Overton, J. Rourke, M. Weller, 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, Julio De Paula. Physical Chemistry, Oxford University Press, Oxford.
- D. A. Mc-Quarie, J .D. Simon. Physical Chemistry: A Molecular Approach, Viva Book Pvt. Ltd.

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

Special Theoretical Papers

CHEM401E: Marks: 50, Credits: 4

Inorganic Special Paper

1. Structure and Properties of Solids (14 Lectures)

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; solid state reactions for synthesis of inorganic materials: ceramic methods, precursor method and sol-gel synthesis, physical and chemical vapour depositions.

2. Supramolecular Chemistry (30 Lectures)

Definition, building block, spacers, atomic and molecular valences; supramolecular orbitals, non-covalent forces: hydrogen bonding, pi-pi and C-H…pi interactions etc. self-assembly: design, synthesis and properties of the self-assembled molecules, self-assembly by H-bonding; catenanes, rotaxanes, dendrimers and supramolecular gels; supramolecular arrays: ribbon, ladder, rack, braded, grid; host-guest interactions**:** synthesis and structures of crown ethers, lariat ethers, podands, cryptands, spherands, calixarene, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands; preorganisation and complimentarity; lock and key analogy, binding of cationic, anionic, ion pair and neutral guest molecules; 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; various types of porous materials, preparation methods, MoF, COF, mesoporous materials and their applications.

3. Isopoly and Heteropoly Acids and Salts (12 Lectures)

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

4. Corrosion (14 Lectures)

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

5. Diffraction Study **(10 Lectures)**

Bravis lattices, space group and its determination, techniques in X-ray structure determination, methods of solving the phase problem, determination of crystal structures.

Reference Books:

- F. A. Cotton, G. Wilkinson, P. L. Gaus. Basic Inorganic Chemistry, 3rd Edn, Wiley India.
- J. E. Huheey, E. A. Keiter, R. L. Keiter. Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edn, Harper Collins 1993, Pearson, 2006.
- B. Douglas, D. McDaniel, J. Alexander. Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons Inc, New York, 2001.
- G. A. Jeffrey. An Introduction to Hydrogen Bonding, Oxford University Press, Oxford, 1997.
- J. W. Steed, J. L. Atwood. Supramolecular Chemistry, 2nd Edn, John Wiley & Sons, New York, 2009.
- R. Martinez-Manez, K. Rurack. 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, D. K. Smith. Supramolecular Chemistry, Oxford University Press, 1999.
- M. Dalal. A Textbook of Inorganic Chemistry - Volume 1, 1st Edn, Dalal Institute, 2017.
- S. Kaya, I. B. Obot, D. Özkir, G. Serdaroglu, A. Singh. Corrosion Science Theoretical and Practical Applications, Apple Academic Press, 2023.
- G. D. Mahan. Many Particle Physics, Kluer Academy, Plenum Publisher, 2000.
- C. Kittel. Introduction to Solid State Physics, John Wiley & Sons, 4th Ed.
- M. F. C. Ladd, R. A. Palmer. Structure Determination by X-ray Crystallography, Plenum Press.
- P. A. Cox. The Electronic Structure & Chemistry of Solids, Oxford University Press, 1987.
- X. Clegg. Crystal Structure Determination, Oxford University Press, 2005.

Organic Special Paper

1. Separation Techniques **(20 Lectures)**

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

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.

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.

2. Heterocyclic Chemistry II **(20 Lectures)**

Synthesis, nomenclature, properties and reactions of the following monocyclic and fused heterocycles:

(i) Azoles: pyrazole, imidazole and oxazoleandthiazole.

(ii) Diazine: pyridazine, pyrimidine and pyrazine.

(iii) Purine, pteridine and folic acid.

ANRORC and Vicarious nucleophilic substitutions in heterocycles;

3. Natural Product II **(15 Lectures)**

Structure, synthesis and reactions of flavonoids and coumarins; reaction and synthesis of steroids (cholesterol, bile acid, testosterone, estrone, progesterone); structure and synthesis of prostaglandins (PGE2, PGF2α)

4. Introduction to Medicinal Chemistry **(25 Lectures)**

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: insulin sensitizers (biguanides, thiazolidine diones), secretagogues (sulfonylureas, nonsulfonyl ureasecretagogues, 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-B complex, vitamin C, vitamin K.

Reference Books:

- T. L. Gilchrist, R. C. Storr. Organic Reactions and Orbital Symmetry, 2nd Edn. Cambridge University Press, 1979.
- R. B. Woodward, 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, A. Yatsimirsky. Principles and Methods in Supramolecular Chemistry, Wiley-VCH, 1999.
- A. T. Kunitake. Supramolecular Chemistry - Fundamentals and Applications, Springer, 2006.
- J. C. Gallagher, C. MacDougall. Antibiotics Simplified, 3rd Edn. Jones and Bartlett Publishers, Inc. 2013.
- C. Walsh. Antibiotics: Actions, Origins, Resistance, Wiley-VCH, 2016.
- S. Sánchez, A. L. Demain. Antibiotics: Current Innovations and Future Trends, Caister Academic Press, 2015.
- B. Testa, U. A. Meyer. Antidiabetic Agents: Recent Advances in Their Molecular and Clinical Pharmacology, Academic Press, 1996.
- K. Chatterjee, E. J. Topol. Cardiac Drugs, Jaypee Brothers Medical Pub. 2013.
- W. H. Frishman, D. A. Sica. Cardiovascular Pharmacotherapeutics, 3rd Edn. Cardio Text, 2011.
- A. Rahman, 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 Paper

1. Approximate Methods and Their Applications (25 Lectures)

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 virial 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, radiation matter interaction, Fermi golden rule, Einstein transition probabilities, lifetime and energy uncertainty.

2. Spin and Many Electron Wave Functions (20 Lectures)

Introduction to spin, operator algebra for spin, construction of matrix representation of spin operators; Eigen values and Eigen functions of spin operators, non-relativistic wave function for hydrogen atom, many-electron wave functions 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 (15 Lectures)

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 (20 Lectures)

Introduction to density functional, Hohenberg-Kohn variation theorem, Kohn-Sham equations, exchange 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-Parr-Pople method, general semi empirical MO methods.

Reference Books:

- L. Pauling, E. B. Wilson. Introduction to Quantum Mechanics, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter, 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, Volume 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, M. Lahmani. Nanomaterials and Nanochemistry, Springer, London, 2006.

CHEM402E: **Marks: 50, Credits: 4**

Inorganic Special Paper

1. Applications of NMR, EPR and Photoelectron Spectroscopy (20 Lectures)

Basic principles of EPR and NMR spectroscopy, background of the spectroscopic tools, selection rules, active chemical systems; elucidation of molecular structures of inorganic compounds from NMR (^{1}H, ^{13}C, ^{11}B, ^{19}F, ^{15}N, ^{17}O, ^{31}P, ^{95}Pt, etc.); structural information of organic radicals and inorganic molecules from EPR spectra; molecular dissymmetry and chiroptical properties; Cotton effect; magnetic circular dichroism (MCD), vibrational circular dichroism (VCD), photoelectron spectroscopy: photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy.

2. Mössbauer Spectroscopy (15 Lectures)

Mössbauer activity: principle, experiment, line-width, center shift, quadrupole interaction, magnetic interaction; information of spin and oxidation states, spin transition from spectra of Mössbauer active nuclei (iron) in variety of environments; 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.

3. Vibrational and Raman Spectroscopy (15 Lectures)

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.

4. Mass Spectrometry (15 Lectures)

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).

5. Electroanalytical Methods II (15 Lectures)

Cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV; methods, choice of solvent, supporting electrolyte, working electrode, switching potential, electrode potential, pathways of electron transfer: EEE, ECE; electro-induced reactions; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn system, electrochemically water oxidation and proton reduction.

References Books:

- D. A .Skoog, F. J. Holler, S. R. Crouch. Instrumental Analysis, Cengage Learning India Pvt. Ltd., New Delhi, 2007.
- H. H. Willard, L. L. Merritt. Jr. J. A. Dean, 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 & Sons Pvt. Ltd. Singapore, 2009).
- G. Currell. Analytical Instrumentation: Performance Characteristics and Quality: (John Wiley and Sons Pvt. Ltd. 2000) Chapter 4.
- E. I. Soloman, A. B. P. Lever. Inorganic Electronic Structure and Spectroscopy, Volume 1, Methodology; Wiley Interscience Publication, 2013.
- C. N. Banwell, E. M. McCash. Fundamentals of Molecular Spectroscopy, 4th Edn, McGraw-Hill, 1994.
- H. Gunther. NMR Spectroscopy, Basic Principles, Concepts and Applications in Chemistry, 3rd Edition, Wiley VCH, 2013.
- S. Glasstone. An Introduction to Electrochemistry, D. Van Nostrand Company, 1962.

Organic Special Paper

1. Supramolecular Chemistry (20 Lectures)

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 **(20 Lectures)**

Asymmetric synthesis: Chiral auxiliaries, substrate, reagent and catalyst controlled reactions; 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 **(20 Lectures)**

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, cis-trans isomerization; 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, radical quenching, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, autooxidation.

4. Oxidation and Reduction of Functional Groups **(20 Lectures)**

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, photo sensitized 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, K. R. Markham. Flavonoids: Chemistry, Biochemistry and Applications, CRC Press, Taylor & Francis, 2006.
- S. K. Talapatra, B. Talapatra. Chemistry of Plant Natural Products, Springer, 2012.
- S. V. Bhat, B. A. Nagasampagi, 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, 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, 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, A. Stolle. Ball Milling Towards Green Synthesis: Applications, Projects, Challenges, Royal Society of Chemistry, 2014.
- R. Cella, H. A. Stefani. Ultrasonic Reactions in Green Techniques for Organic Synthesis and Medicinal Chemistry, John Wiley & Sons, Ltd, Chichester, UK, 2012.
- K. Tanka. Solvent-free Organic Synthesis, 2nd Edn, Wiley-VCH, 2009.
- V. K. Ahluwalia, M. Kidwai. New Trends in Green Chemistry, Springer, 2004.
- N. J. Turro. Modern Molecular Photochemistry, Benjamin/Cummings Publishing Co. Inc. 1978.
- R. B. Woodward, R. Hoffman. The Conservation of Orbital Symmetry, Academic Press, 1970.
- J. M. Coxon, B. H. Halton. Organic Photochemistry, Cambridge University Press, 1974.

Physical Special Paper

1. Excitation of Molecules and Motion in Excited State (10 Lectures)

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 (15 Lectures)

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 (25 Lectures)

Atomic structure: vector model, spin-orbit coupling, atomic states, 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, photo-dissociation, pre-dissociation, 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 (20 Lectures)

Nuclear magnetic moment, classical and quantum mechanical perspectives of nuclear magnetic resonance (NMR), Bloch equations, spin-spin and spin-lattice relaxation, spectral shapes, free induction decay, FT-NMR technique; chemical shift and nuclear shielding; spin magnetic moment of electrons, electron spin resonance (ESR) signal, the g-factor, hyperfine splitting-interaction between nuclear spin and electron spin, multi-dimensional NMR spectroscopy, nuclear quadruple resonance; applications and instrumentation of NMR and ESR.

5. Advanced Techniques in Spectroscopy and Microscopy (10 Lectures)

Time resolved fluorescence spectroscopy, principles of instrumentation, data analysis; single molecule fluorescence, fluorescence correlation spectroscopy, fluorescence lifetime imaging; optical tweezers.

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, B. K. Hunter. Modern NMR Spectroscopy: A Workbook of Chemical Problems, Oxford University Press, Oxford, 1993.
- C. N. Banwell, 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, 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, H. O. Willis. Computer Methods in Ultraviolet, Visible and Infra-red Spectroscopy, 1989.

CHEM403E: **Marks: 50, Credits: 4**

Inorganic Special Paper

1. Organometallic Chemistry II (15 Lectures)

Reactions that occur at the metal: ligand substitution, oxidative addition, reductive elimination; reactions involving modification of ligands: insertion and deinsertion, nucleophilic addition to the ligand, nucleophilic abstraction, electrophilic reactions; applications to organic synthesis: enantioselective functional group interconversion, chiral synthesis, protection and deprotection; transmetallation and cyclisation reactions, metallo-fullerenes, bioorganometallics, organo-lanthanoids and actinoids, organodendrimer, surface organometallic chemistry.

2. Inorganic Reaction Mechanism II (20 Lectures)

Mechanism of isomerization reaction-linkage 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., Trans effect, cis effect, outer-sphere reaction, inner-sphere reaction, effect of bridging ligand in inner-sphere reaction, kinetics and mechanism, electron tunneling hypothesis, heteronuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its applications, 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.

3. Molecular Magnetism II **(15 Lectures)**

Isolation of different molecular magnets, magnetic interactions in di- and polynuclear systems and clusters, cryogenic experiment, mechanism of exchange interaction, Bleaney-Bowers equation, anti ferromagnetism (AF), ferromagnetism (F), single molecule magnet, deliberate synthetic approach of ferromagnetically coupled system, accidental orthogonality, spin canting, canted-AF, canted-F, spin frustration, admixed-spin, spinflop, metamagnetism, superparamagnetism, long-range ordering, calculation of ground state and spin manifold, magnetization versus field studies, inorganic, organic, metal-organic and organometallic magnetic materials.

4. Metals in Medicine **(15 Lectures)**

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, photodynamic therapy (PDT), nuclear medicine, MRI contrast agents.

5. Nano Science **(15 Lectures)**

Preparation of nano particles: top down and bottom up approach, electrochemical, chemical, photo-chemical and biochemical synthesis of nano particles; properties of nano particles, variation of properties with size; scanning probe microscopy (SPM): introduction, basic principles of SPM techniques; the details of STM, summary of STM; general concept and defining characteristics of AFM; electron microscopy: introduction, resolution vs magnification; scanning electron microscope (SEM): techniques; electronGun, specimen interactions, energy dispersive X-ray analysis, environmental SEM; transmission electron microscope (TEM); bright field image mode, dark field image mode, high resolution TEM; applications of nano particles.

Reference Books:

- P. Powell. Principles of Organometallic Chemistry, 2nd Edn, Chapman and Hall, London, 1988.
- J. D. Atwood. Inorganic and Organometallic Reaction Mechanisms, 2nd Edn, VCH, New York, 1997.
- R. H. Crabtree. The Organometallic Chemistry of the Transition Metals, 4th Edn, Wiley, New York, 2005.

- C. Elschenbroich. Organometallics, 3rd Edn, Wiley-VCH, Weinheim, 2006.
- R. A. van Santen, M. Neurock. Molecular Heterogenous Catalysis, Wiley-VCH, Weinheim, 2006.
- G. O. Spessard, G. L. Miessler. Organometallic Chemistry, International 2nd Edn, Oxford University Press, Oxford, 2010.
- J. F. Hartwig. Organotransition Metal Chemistry. From Bonding to Catalysis, University Science Books, Sausalito, CA, 2010.
- R. G. Wilkinns. Kinetics and Mechanism of Reactions of Transition Metal Complexes, 2nd Edn, VCH, Weinheim, 1991.
- J. O. Edwards, W. A. Benjamin. Inorganic Reactions Mechanism, INC, New York, 1965.
- C. H. Langford, H. B. Gray. Ligand Substitution Processes, W. A. Benjamin, New York, 1966.
- F. Basolo, R. G. Pearson. Mechanism of Inorganic Reactions, 2nd Edn, Wiley, New York, 1967.
- D. Katakis, G. Gordon. Mechanisms of Inorganic Reactions, John Wiley & Sons, New York, 1987.
- R. L. Carlin. Magnetochemistry, Springer-Verlag, New York, 1986.
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- P. M. Lathi. Magnetic Properties of Organic Materials, Marcel Dekker, New York, 1999.
- J. S. Miller, M. Drillon. Magnetism: Molecules to Materials, V; Molecule-based Magnets, Wiley-VCH, Weinheim, 2005.
- P. Gutlich, H. A. Goodwin. Spin Crossover in Transition Metal Compounds, Springer, Berlin, 2004.
- F. E. Mabbs, D. J. Machin. Magnetism and Transition Metal Complexes, Dover Publications, 2008.
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- D. Gatteschi, R Sessoli, J. Villain. Molecular Nanomagnets, Oxford University Press, Oxford, 2006.
- R. Hilzinger, W. Rodewald. Magnetic Materials, Wiley, New York, 2013.
- C. M. Sorensen. Magnetism in Nanoscale Materials in Chemistry, Wiley Interscience, New York, 2001.
- Medicinal Inorganic Chemistry, Edited by J. L. Sessler, S. R. Doctrow, T. J. McMurry, S. J. Lippard. American Chemical Society, Washington, DC.
- Radiopharmaceutical Chemistry, Jason S. Lewis, Albert D. Windhorst, Brian M. Zeglis, Springer, 2019.
- B.W. Henderson, T.J. Daugherty. Photodynamic Therapy: Basic Principles and Clinical Applications, 1st Edn, 1992.
- Chad A. Mirkin, Christ of M. Niemeyer. Nanobiotechnology II: More Concepts and Applications 2007, Wiley-vch Verlag Gmbh.
- C.P. Poole, F.J. Owens. Introduction to Nanotechnology, Wiley India, 2006.
- G. A. Ozin, C. Andre, L. Arsenault. Cademartiri, Nanochemistry: A chemical Approach to Nanomaterials, Royal Society of Chemistry, 2005.
- T. Pradeep, NANO: The Essentials, Tata-McGraw Hill, New Delhi, 2007.
- K. J. Klabunde, Nanoscale Materials in Chemistry, Wiley-interscience, 2001.
- Bharat Bhushan (Ed.) Springer Handbook of Nanotechnology, Springer, 2007.

Organic Special Paper

1. Protein and Lipid **(20 Lectures)**

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.

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

2. Nucleic acid and Enzymes **(30 Lectures)**

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; nucleosides and nucleotides.

Enzymes: Nomenclature and classification, extraction (large scale production) and purification

of 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.

Mechanism in biological chemistry: 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 thiaminphosphate; chemical synthesis of peptides and proteins; use of enzymes in organic synthesis; structural analysis of proteins; protein folding.

3. Carbohydrates (20 Lectures)

Basic structures and types of sugar, reaction: protection and deprotection, deoxy-sugar, amino sugar; glycol sugars and their synthetic aspect; 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 (10 Lectures)

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, J. Michl. Excited States and Photo-Chemistry of Organic Molecules, Wiley, 1995.
- S. V. Bhat, B. A. Nagasampagi, M. Sivakumar. Chemistry of Natural Products, Narosa Publishing House, New Delhi, 2005.
- X.-T. Liang, W.-S. Fang. Medicinal Chemistry of Bioactive Natural Products, John Wiley & Sons, 2006.
- T. Hudlicky, 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 of Natural Products, 5^{th} Edn, Pearson Education India, 1956.
- G. C. Howard, 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 Paper

1. Connection between Thermodynamics and Statistical Mechanics (10 Lectures)

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 Applications (20 Lectures)

Definition of ensemble, A priori probability, Gibbs postulate in statistical mechanics, Ergodic hypothesis; study 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 (30 Lectures)

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 electronic 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 (20 Lectures)

The classical partition function, phase space, 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.

CHEM404C: Marks: 50, Credits: 4

Medicinal Chemistry

1. Medicinal Chemistry and Drug Discovery: (10 Lectures)

Antibacterial, anticancer, antitussive, antiviral agents; opium analgesics, antibiotics; new drugs from old poisons; drug discovery; structure-activity relationships (SARs)

2. Radiopharmaceuticals: (30 Lectures)

Nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; type of radionuclides, neutral/charged particle emitters, radionuclide generators; ideal radiopharmaceuticals, methods of radiolabeling, biodistribution, specific radiopharmaceuticals for diagnostic and therapeutic purposes, SPECT, PET, 18FDG, method of administration, principle and instrumentation of gamma/PET camera for detection, quality control, principle, method and application of radioimmuassay (RIA).

3. Medicinal Inorganic Chemistry: (15 Lectures)

Biomedical significance and inorganic chemistry, characterization of biomolecules using spectroscopic methods, mechanistic aspects of heavy metal toxicity, platinum anti-cancer drugs (from laboratory to clinic), discovery and development of newer generation anti-tumour and anti-cancer agents.

4. Pharmacokinetics: (10 Lectures)

Drug absorption, drug distribution, drug metabolism, drug excretion, drug administration, drug dosing.

5. Photodynamic Medicine: (15 Lectures)

Introduction, early days of photodynamic therapy (PDT), basic principle, photodynamic action,

photochemotherapy, photosensitizing molecule, incubation period, light activation, light exposure, total light dose and its fluence rate, application of photosensitizer drug.

Reference Books:

- J. S. Lewis, A. D. Windhorst, B. M. Zeglis. Radiopharmaceutical Chemistry, Springer, 2019**.**
- B. W. Henderson, T. J. Daugherty. Photodynamic Therapy: Basic Principles and Clinical Applications, 1st Edn, CRC Press, 1992.
- A. Dash, F. F. Knapp. Radiopharmaceuticals for Therapy, Springer, 2016.
- A. Owunwanne, M. Patel, S. Sadek. The Handbook of Radiopharmaceuticals, Chapman & Hall Medical, 1st Edn, 1995.
- M. J. Welch, C. S. Redvanly. Handbook of Radiopharmaceuticals: Radiochemistry and Applications, Wiley, 2005.
- An Introduction to Medicinal Chemistry, Graham L. Patrick. Oxford International Student Edition.
- J. L. Sessler, S. R. Doctrow, T. J. McMurry, S. J. Lippard. Medicinal Inorganic Chemistry, American Chemical Society, Washington, DC.
- G. Patrick. Instant Notes on Medicinal Chemistry, Viva Books Pvt. Ltd.
- F. D. King. Medicinal Chemistry, Principles and Practice, Royal Society of Chemistry.
- C. G. Wermuth. The Practice of Medicinal Chemistry, Academic Press.

CHEM 405E (PR): **Marks: 50, Credits: 4**

Inorganic Special Practical

1. Preparation of inorganic complexes
   (i) Using synthesized bi-, tri- and poly-dentate N, O, S donor ligands.
   (ii) Synthesis under inert atmosphere, electro-synthesis and their characterization.
   (a) FTIR, ESI-Mass and NMR spectroscopy.
   (b) Elemental Analysis (C, H, N and S or other analytical methods).
   (c) Growing of single crystals and their X-ray diffraction studies.
   (d) Spectral, thermal, electrochemical and magnetic studies.
2. Kinetic and mechanistic studies of some selected reactions (substitution and redox).
3. Chromatographic and ion-exchange separation of ions and molecules.
4. Visit to research institute/industry.

Reference Books:

- G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney. Vogel's Textbook of Quantitative Chemical Analysis. 5th Edn. John Wiley & Sons, New York, 1989.

- G. N. Mukherjee. Advanced Experiments in Inorganic Chemistry, 2nd Edn. U. N. Dhur & Sons Pvt. Ltd. 2018.
- Dr. L. R. Sharma. Practical Inorganic Chemistry, Evincepub Publishing, 2021.

Organic Special 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 characterization by recrystallisation, chromatographic separation (as applicable), determination of mp/bp (as the case may be), and spectral measurements (UV, IR, ESI-MS, NMR) (model experiments/reactions/compounds).

- Beckmann rearrangement: benzanilide from benzene. (benzene to benzophenone to benzophenone oxime to benzanilide).
- Synthesis of 1-phenyl-3-methyl-5-pyrazolone from phenyl hydrazine.
- Synthesis of 2-phenylindole from phenyl hydrazine.
- Preparation involving chlorosulphonation.
- Preparation involving Friedel-Crafts reaction.
- Preparation involving diazo-coupling reaction.
- Preparation involving Reimer-Tiemann reaction.
- Coumarin ring synthesis.
- Preparation of 4-hydroxy-6-methyl-2-pyrone.

(At least five experiments to be carried out during lab session.)

2. Visit to research institute/industry.

Reference Books:

- B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell. Vogel's Textbook of Practical Organic Chemistry, 5th Edn. John Wiley & Sons. New York, 1989.
- A. I. Vogel. A Textbook of Practical Organic Chemistry, 3rd Edn. Longman Group Ltd. London, 1956.
- R. C. Bhattacharyya. A Manual of Practical Chemistry, 11th Edn. Studies book sellers & publishers, Calcutta, 1992.
- Roberts, Gilbert, Rodewaid, Wingrove. An Introduction to Experimental Organic Chemistry, 3rd Edn. Holt, Rinehart & Winston Publishers, New York, 1969.
- H. T, Clarke. Handbook of Organic Analysis, 4th Edn. Hodder & Stoughton Educational, London, 1926.

- H. Middleton. Systematic Qualitative Organic Analysis, 2nd Edn. Hodder & Stoughton Educational, London, 1943.
- V. K. Ahluwalia, R. Aggarwal. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press, 2001.
- E. Stahl. Thin Layer Chromatography, 2nd Edn. Springer, 1969.
- R. M. Silverstein. Spectrometric Identification of Organic Compounds, 6th Edn. John Wiley & Sons, New York, 1997.

Physical Special Practical

- To determine the effect of change of (i) temperature and (ii) concentration on the rate constant of hydrolysis of an ester.
- To study the conductance behavior of strong and weak electrolytes.
- To determine the CMC of SDS in water and water-ethanol (1:1) mixture using conductometry.
- To determine the hydrolysis constant of aniline hydrochloride by conductometry.
- To study the titration of H_3PO_4 by NaOH using potentiometry.
- To determine the concentration of different halides in a mixture by potentiometry.
- 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.
- To determine the order and rate constant of the reaction between $HBrO_3$ and HI.
- Visit to research institute/industry.

Reference Books:

- B. Viswanathan, P. S. Raghavan. Practical Physical Chemistry, Viva Books, 2009.
- J. Mendham. Vogel's Quantitative Chemical Analysis, 6th Edn. Pearson Education, 2009.
- D. C. Harris. Quantitative Chemical Analysis, 6th Edn. W. H. Freeman, 2007.
- S. R. Palit, S. K. De. Practical Physical Chemistry, Science Book Agency.
- University Hand Book of Undergraduate Chemistry Experiments, edited by G. N. Mukherjee. University of Calcutta.
- B. P. Levitt. Findlay's Practical Physical Chemistry, 9th Edn. Longman Group Ltd. 1973.
- J. N. Gurtu, R. Kapoor. Advanced Experimental Chemistry, S. Chand & Co. Ltd.