

MASTER OF SCIENCE IN CHEMISTRY
TWO YEARS FULL TIME PROGRAMME

RULES, REGULATIONS AND COURSE CONTENTS



DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCE
UNIVERSITY OF DELHI
DELHI – 110007

2018

MASTER OF SCIENCE IN CHEMISTRY

TWO YEARS FULL TIME PROGRAMME

AFFILIATION

The proposed programme shall be governed by the Department of Chemistry, Faculty of Science, University of Delhi, Delhi – 110007.

PROGRAMME STRUCTURE

The Master of Science in Chemistry course is a Two Year Full Time Course consisting of four semesters, to be known as Semester I, Semester II, Semester III and Semester IV.

Part I	First Year	Semester I	Semester II
Part II	Second Year	Semester III	Semester IV

COURSE STRUCTURE

Semester	Core courses			Elective courses			Open elective courses			Total credits
	No. of papers	Credits (L+T/P)	Total credits	No. of papers	Credits (L+T/P)	Total credits	No. of papers	Credits (L+T/P)	Total credits	
I	3	12 + 6(P)	18	0	0	0	0	0	0	18
II	3	12 + 6(P)	18	0	0	0	0	0	0	18
III	3	12	12	1(P)	8(P)	8	1	4	4	24
IV	0	0	0	4+1(P)	16 + 8(P)	24	0	0	0	24
Total credits for the course			48			32			4	84

N.B.: **80 credits as core/elective courses** and **4 credits as open elective course** are compulsory to obtain the M.Sc. degree.

Semester-wise Course Details

Semester I				
Number of core courses	Six (3 Theory + 3 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core course 1	4	2	0	6
Core course 2	4	2	0	6
Core course 3	4	2	0	6
Total credits in core course				18
Number of elective courses	Nil			
Total credits in elective course				0
Total credits in Semester I				18

Semester II				
Number of core courses	Six (3 Theory + 3 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core course 4	4	2	0	6
Core course 5	4	2	0	6
Core course 6	4	2	0	6
Total credits in core course				18
Number of elective courses	Nil			
Total credits in elective course				0
Total credits in Semester II				18

Semester III				
Number of core courses	Three (3 Theory)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core course 7	4	0	0	4
Core course 8	4	0	0	4
Core course 9	4	0	0	4
Total credits in core course				12
Number of elective courses	One (1 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Elective practical 1	0	8	0	8
Total credits in elective course				8
Number of open electives	One			
	Credits in each open elective			
	Theory	Practical	Tutorial	Total
Open elective 1	4	0	0	4
Total credits in open elective				4
Total credits in Semester III				24

Semester IV				
Number of core courses	Nil			
Total credits in core course	0			
Number of elective courses	Four (3 Theory + 1 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Elective course 1	4	0	0	4
Elective course 2	4	0	0	4
Elective course 3	4	0	0	4
Elective course 4	4	0	0	4
Elective practical 2 and Research Project	0	8	0	8
Total credits in elective course	24			
Total credits in Semester IV	24			
Total credits of the course = 18 + 18 + 24 + 24 = 84				

MASTER OF SCIENCE IN CHEMISTRY COURSE

Examination and Scheme of Papers

- (i) The duration of the course for the degree of Master of Science in Chemistry shall be two academic years.
- (ii) All the papers listed below are to be taught in two parts (Courses A and B).
- (iii) The course is divided into four semesters and there shall be an examination at the end of each semester as given below:

Scheme of Papers

Part I

Semester I

<i>Paper No.</i>	<i>Title</i>	<i>Duration of Examination (Hours)</i>	<i>Maximum Marks</i>	<i>Credits</i>
Paper 101	Inorganic Chemistry – I <i>Stability Constants of Metal Complexes and Their Applications / Supramolecular and Photoinorganic Chemistry</i> (Core course 1)	3	100	4
	Inorganic Chemistry – I (Practical core course 1)	Continuous Evaluation	50	2
Paper 102	Organic Chemistry – I <i>Reactive Intermediates in Organic Chemistry / Stereochemistry of Organic Compounds</i> (Core course 2)	3	100	4
	Organic Chemistry – I (Practical core course 2)	Continuous Evaluation	50	2
Paper 103	Physical Chemistry – I <i>Quantum Chemistry/Mathematical Methods</i> (Core course 3)	3	100	4
	Physical Chemistry – I (Practical core course 3)	Continuous Evaluation	50	2
TOTAL			450	18

Semester II

<i>Paper No.</i>	<i>Title</i>	<i>Duration of Examination (Hours)</i>	<i>Maximum Marks</i>	<i>Credits</i>
Paper 201	Inorganic Chemistry – II <i>Group Theory and its Applications / Chemistry of d-and f-block Elements</i> (Core course 4)	3	100	4
	Inorganic Chemistry – II (Practical core course 4)	Continuous Evaluation	50	2
Paper 202	Organic Chemistry – II <i>Spectroscopy of Organic Compounds / Reagents and Methods of Organic Synthesis</i> (Core course 5)	3	100	4
	Organic Chemistry – II (Practical core course 5)	Continuous Evaluation	50	2
Paper 203	Physical Chemistry – II <i>Statistical Mechanics & Thermodynamics, Electrochemistry, Kinetics and Macromolecules</i> (Core course 6)	3	100	4
	Physical Chemistry – II (Practical core course 6)	Continuous Evaluation	50	2
TOTAL			450	18

Note: Each of the Practical Chemistry Papers shall be based on continuous evaluation. 25% of the total marks for the Practical shall be reserved for the Laboratory Record/ Sessional Work of the candidates and 15% marks for viva-voce.

30 marks (24 marks for internal exam and 6 marks for attendance) in each theory paper are reserved for internal assessment.

Part II**Semester III**

Paper No.	Title	Duration of Examination (Hours)	Maximum Marks	Credits
Paper 301	Inorganic Chemistry – III <i>Inorganic Reaction Mechanisms / Catalysis and Bio-inorganic Chemistry</i> (Core course 7)	3	100	4
Paper 302	Organic Chemistry – III <i>Photochemistry & Pericyclic Reactions / Medicinal Chemistry</i> (Core course 8)	3	100	4
Paper 303	Physical Chemistry – III <i>Molecular Structure: Spectroscopic and Diffraction Methods</i> (Core course 9)	3	100	4
Paper 3101 [*]	Inorganic Chemistry (Special - I) <i>Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds / Introduction to the Solution of Multielectron Problems</i> (Open Elective-1)	3	100	4
Paper 3102 [*]	Inorganic Chemistry (Special - II) <i>Introduction to Nanochemistry</i> (Open Elective-1)	3	100	4
Paper 3201 [#]	Organic Chemistry (Special - I) <i>Chemistry of Life Processes & Bioactive Compounds</i> (Open Elective-1)	3	100	4
Paper 3202 [#]	Organic Chemistry (Special-II) (Open Elective-1) <i>Polymer Chemistry & Processing and Role of Catalysis in Chemical Synthesis</i>	3	100	4
Paper 3301 ^a	Physical Chemistry (Special - I) <i>Irreversible Thermodynamics, Transport Phenomena, Surface Phenomena & Fast Reactions</i> (Open Elective-1)	3	100	4
Paper 3103	Practical Inorganic Chemistry - I (Elective practical 1)	Continuous evaluation	200**	8
Paper 3203	Practical Organic Chemistry – I (Elective practical 1)	Continuous evaluation	200**	8
Paper 3302	Practical Physical Chemistry – I (Elective practical 1)	Continuous evaluation	200**	8

*Inorganic Chemistry Section will offer either Paper 3101 or 3102 as Open elective.

#Organic Chemistry Section will offer either Paper 3201 or 3202 as Open elective

^aPrerequisite: mathematics upto the +2 level for Paper 3301.

**The Practical Paper in each branch in Semester III shall be continuously evaluated.

25% of the marks will be reserved for the Laboratory Record/ Sessional work of the candidates and 15% marks for viva-voce.

Semester IV

(1) Inorganic Group:

Paper No.	Title	Duration of Examination (Hours)	Maximum Marks	Credits
Paper 4101	Inorganic Chemistry (Special - III) <i>Spectral Techniques in Inorganic Chemistry</i> (Elective course 1)	3	100	4
Paper 4102	Inorganic Chemistry (Special - IV) <i>Organotransition Metal Chemistry / Bio-inorganic Chemistry</i> (Elective course 2)	3	100	4
Paper 4103	Inorganic Chemistry (Special - V) <i>Analytical Techniques</i> (Elective course 3)	3	100	4
Paper 4104	Inorganic Chemistry (Special - VI) <i>Materials / Nuclear and Radiochemistry</i> (Elective course 4)	3	100	4
Paper 4105	Inorganic Chemistry (Special - VII) <i>Green Chemistry: An interdisciplinary approach towards sustainable development</i> (Elective course 4)	3	100	4
Paper 4106	Practical Inorganic Chemistry – II Practical & Research Project Evaluation (Elective practical 2)	Continuous evaluation	200 [#]	8

*Inorganic Chemistry Section will offer either Paper 4104 or 4105 as 4th elective.

[#]100 marks are reserved for practicals (continuous evaluation). 25% of these marks will be reserved for the Laboratory Record/ Sessional work of the candidates and 15% marks for viva-voce. The remaining 100 marks are reserved for the Research Project, which includes submitting a dissertation and making a presentation.

(2) Organic Group:

Paper No.	Title	Duration of Examination (Hours)	Maximum Marks	Credits
Paper 4201	Organic Chemistry (Special - II) <i>Advanced Organic Synthesis / Supramolecular Chemistry and Carbocyclic Rings</i> (Elective course 1)	3	100	4
Paper 4202	Organic Chemistry (Special - III) <i>Terpenes and Steroids / Alkaloids and Polyphenols</i> (Elective course 2)	3	100	4
Paper 4203	Organic Chemistry (Special - IV) <i>Newer Synthetic Reactions and Reagents / Heterocyclic Chemistry</i> (Elective course 3)	3	100	4
Paper 4204	Organic Chemistry (Special - V) <i>Biomolecules</i> (Elective course 4)	3	100	4
Paper 4205	Organic Chemistry (Special - VI) <i>Pharmaceutical Techniques Technologies Development</i> (Elective course 4)	3	100	4
Paper 4206	Practical Organic Chemistry – II & Research Project Evaluation (Elective practical 2)	Continuous evaluation	200 [#]	8

*Organic chemistry section will offer either Paper 4204 or 4205 as 4th elective.

^{##} 100 marks are reserved for practicals (continuous evaluation). 25% of these marks will be reserved for the Laboratory Record/ Sessional work of the candidates and 15% marks for viva-voce. The remaining 100 marks are reserved for the Research Project, which includes submitting a dissertation and making a presentation.

(3) *Physical Group:*

<i>Paper No.</i>	<i>Title</i>	<i>Duration of Examination (Hours)</i>	<i>Maximum Marks</i>	<i>Credits</i>
Paper 4301	Physical Chemistry Special <i>Advanced Statistical Mechanics</i> (Elective)	3	100	4
Paper 4302	Physical Chemistry Special <i>Advanced Electrochemistry</i> (Elective)	3	100	4
Paper 4303	Physical Chemistry Special <i>Advanced Photochemistry & Radiation Chemistry</i> (Elective)	3	100	4
Paper 4304	Physical Chemistry Special <i>Computational Methods in Chemistry</i> (Elective)	3	100	4
Paper 4305	Physical Chemistry Special <i>Advanced Quantum Chemistry</i> (Elective)	3	100	4
Paper 4306	Physical Chemistry Special <i>Advanced Chemical Kinetics</i> (Elective)	3	100	4
Paper 4307	Physical Chemistry Special <i>Advanced Molecular Spectra</i> (Elective)	3	100	4
Paper 4308	Physical Chemistry Special <i>Crystal Structure</i> (Elective)	3	100	4
Paper 4309	Physical Chemistry Special <i>Macromolecules</i> (Elective)	3	100	4
Paper 4310	Physical Chemistry Special <i>Biophysical Chemistry</i> (Elective)	3	100	4
Paper 4311	Physical Chemistry Special <i>Physical Chemistry of Materials</i> (Elective)	3	100	4
Paper 4312	Practical Physical Chemistry - II & Research Project Evaluation. (Elective)	Continuous evaluation	200**	8
	GRAND TOTAL (M.Sc. Course)		2100	84
<p><i>Note: Papers belonging to physical chemistry teaching in semester-IV may combine any two parts, viz. course A or course B, of same or different elective papers (4301 to 4311). These combined courses will form 4 elective papers.</i></p>				

**100 marks are reserved for practicals (continuous evaluation). 25% of these marks will be reserved for the Laboratory Record/ Sessional work of the candidates and 15% marks for viva-voce. The remaining 100 marks are reserved for the Research Project, which includes submitting a dissertation and making a presentation.

Notes:

- (1) At the beginning of Semester III, the students will be required to choose their specialization, viz. Inorganic, Organic or Physical Chemistry and take Elective papers accordingly. They will take one Special Paper (Open elective 1) in Semester III and four Papers of the specialization of their choice or, alternatively, three special papers (Electives) of the specialization of their choice and one paper out of the open elective papers offered by their specialization or other Science Departments in Semester III. They will also have to take two Special Practical Papers (Elective practicals, one each in Semester III and IV). For Physical Chemistry (Special) Semester IV, the options available as Electives and the elective (from among Physical Chemistry Special Papers 4301 - 4311) will be notified at the Chemistry Department website before the session starts. Mathematics upto at least the +2 level is a prerequisite for the Physical Chemistry Open Electives.
- (2) *The two Practical Papers in each branch in Semesters III and IV shall be continuously evaluated. 25% of the marks will be reserved for the Laboratory Record/ Sessional work of the candidates and 15% marks for viva-voce. In Semester IV, the practical marks will be divided between practicals (100 marks) and Research Project (100 marks).
- (3) 30 marks (24 marks for internal exam and 6 marks for attendance) in each theory paper are reserved for internal assessment.
- (4) Mathematics upto the +2 level is a prerequisite for Open Electives from Physical Chemistry.

SCHEME OF EXAMINATIONS

1. English shall be the medium of instruction and examination.
2. Examinations shall be conducted at the end of each Semester as per the Academic Calendar notified by the University of Delhi.
3. The system of evaluation shall be as follows:
 - 3.1 Each course will carry 100 marks, of which 30 marks shall be reserved for internal assessment based on classroom participation, seminar, term courses, tests and attendance. The weightage given to each of these components shall be decided and announced at the beginning of the semester by the individual teacher responsible for the course. Any student who fails to participate in classes, seminars, term courses, tests, will be debarred from appearing in the end-semester examination in the specific course and no Internal Assessment marks will be awarded. His/her Internal Assessment marks will be awarded as and when he/she attends regular classes in the course in the next applicable semester. No special classes will be conducted for him/her during other semesters.
 - 3.2 The remaining 70 marks in each paper shall be awarded on the basis of a written examination at the end of each semester. The duration of the written examination for each paper shall be three hours.
 - 3.3 A candidate is allowed to reappear ONLY in THEORY papers to improve his/her previous performance.
4. Examinations for courses shall be conducted only in the respective odd and even semesters as per the Scheme of Examinations. Regular as well as Ex-Students shall be permitted to appear/ re-appear/ improve in courses of Odd Semesters only at the end of Odd Semesters and courses of Even Semesters only at the end of Even Semesters.

PASS PERCENTAGE

- Minimum marks for passing the examination in each semester shall be 40% in each paper and 45% in the aggregate of a semester.
- No student would be allowed to avail of more than 3 chances to pass any paper, inclusive of the first attempt.

CRITERIA FOR PROMOTION AND AWARD OF DEGREE

- For promotion from Part I to Part II, the student must pass at least 4 theory papers and also the practical examination (pass percentage 40%).
- A candidate will be awarded the M.Sc. degree at the end of Semester IV, provided he / she has passed all theory papers of Part – I and Part – II and practicals, separately, by securing at least 40% marks in each paper.

DIVISION CRITERIA

Successful candidates will be classified on the basis of the combined results of Part-I and Part-II examinations as follows:

Candidates securing 60% and above	:	I st Division
Candidates securing between 50% and 59.99%	:	II nd Division
All others (securing between 40% and 49.99%)	:	Pass

SPAN PERIOD

No student shall be admitted as a candidate for the examination for any of the Parts/ Semesters after the lapse of 4 years from the date of admission to Part-I/ Semester-1 of the M. Sc. Chemistry Programme.

ATTENDANCE REQUIREMENT

No student shall be considered to have pursued a regular course of study unless he/ she is certified by the Head, Department of Chemistry, University of Delhi, to have attended 75% of the total number of lectures, tutorials and seminars conducted in each semester, during his/ her course of study. Provided that he/ she fulfils other conditions, the Head, Department of Chemistry, may permit a student who falls short of the required percentage of attendance by not more than 10 per cent of the lectures, tutorials and seminars conducted during the semester, to the next Semester.

DETAILED COURSES

M. Sc. PART I

SEMESTER – I

Paper 101- Inorganic Chemistry-I (Core course I) (100 Marks/ 4 Credits)

Course A: Stability constants of metal complexes and their applications

Stoichiometric and thermodynamic equilibrium constants, stepwise formation of complexes, formation functions, φ , β and α_C and relationship between different functions. Calculation of stability constants. Graphical Methods: using sets of data $\{\varphi, [A]\}$; $\{\alpha_C, [A]\}$ and $\{\beta, [A]\}$.

Curve fitting method, Elimination method, Numerical method, Potentiometric method, Method of corresponding solutions, Ion exchange method, Solvent extraction, Polarographic method and Spectrophotometric methods, which include Job's method of continuous variation, Logarithmic method, Bent and French mole ratio method. Turner and Anderson methods and Yatsimirskiis method.

Analytical applications of complex formation; gravimetric analysis, complexometric titrations (Conditional constants, titration curves, titration error, detection of end point using metal indicators and instrumental methods. Indicator errors, Indicator correction, etc. Simultaneous titrations, stepwise titrations, back titrations). Use of masking and demasking agents in complexometric titrations.

Course B: Supramolecular and Photoinorganic Chemistry

Introduction: Molecules and Supramolecules, Supermolecules, Large Molecules Classification, Nomenclature, Thermodynamic and Kinetic selectivity, Supramolecular interactions, Supramolecular host design, Macrocyclic versus acyclic hosts, Chelate Macrocyclic and macrobicyclic hosts, High dilution synthesis, Template synthesis

Molecular recognition: Receptors, design and synthesis of co-receptors and Multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules.

Redox reactions of metal complexes in excited states, excited electron transfer, examples using $[\text{Ru}(\text{bpy})_3]^{2+}$ complex and $[\text{Fe}(\text{bpy})_3]^{3+}$ complex. Role of spin-orbit coupling, life-times of excited states in these complexes.

Metal complex sensitizers: Electron relay, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO_2 reduction.

Recommended Texts:

1. Christian, G. D., Analytical Chemistry, 6th Ed., John Wiley & Sons, Inc. (2004).
2. Khopkar, S.M., Basic Concepts of Analytical Chemistry 3rd Edition, Publisher: New Age International Publishers (2008), ISBN: 9788122420920, 8122420923.
3. Eldik, R. V.; Stochel G. Advances in Inorganic Chemistry: Inorganic Photochemistry, Volume 63, 1st Edition, Academic Press (2011)
4. Hartley, F. R., Burgess, C. & Alcock, R. M. *Solution Equilibria*. Prentice-Hall: Europe (1980).
5. Atwood, J. L. & Steed, J. W. *Supramolecular Chemistry: A Concise Introduction* John Wiley & Sons (2000).
6. Lehn, J. M. *Supramolecular Chemistry: Concepts & Perspectives*, Print ISBN:9783527293124 Wiley-VCH (2006).
7. Desiraju, G. R., Ed. *Perspectives in Supramolecular Chemistry*, Vol. 2: *Crystal Engineering and Molecular Recognition* Wiley: Chichester (1995).

8. Srivastava and Mishra, Fundamental of Analytical Chemistry (First Edition, 2016)
9. Robinson, J.W, Undergraduate Instrumental Analysis, CRC Press (2014).
10. Inczedy, J. *Analytical applications of complex equilibria* Halsted Press: New York, NY (1976).

Practical core course 1 (50 Marks/ 2 credits)

Inorganic Chemistry - 101

1. Quantitative analysis of mixtures of metal ions by complexometric titrations (mixture of two metals) with the use of masking and de-masking agents.
2. Any other experiments done in the class during the semester.

Paper 102- Organic Chemistry-I (Core course 2) (100 Marks/ 4 Credits)

Course A: Reactive Intermediates in Organic Chemistry

A review of reaction mechanisms including methods of determination.

Linear free energy relationships and their applications (Hammett equation and modifications).

Carbocations: Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.

Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.

Free Radicals: Generation, structure, stability and reactions, cage effects; radical-cations & radical-anions, $S_{RN}1$ mechanisms.

Carbenes: Formation and structure, reactions involving carbenes and carbenoids.

Nitrenes: Generation, structure and reactions of nitrenes.

Arynes: Generation and reactivity of arynes, nucleophilic aromatic substitution reactions, $S_{N}Ar$ mechanism; Ipsso effect.

Course B: Stereochemistry of Organic Compounds

Molecular symmetry and chirality: Symmetry operations and symmetry elements, point group classification and symmetry number.

Stereoisomerism: Classification, racemic modification, molecules with one, two or more chiral centres; Configuration nomenclature, D L, R S and E Z nomenclature. Axial and planar chirality and helicity (P & M); Stereochemistry and configurations of allenes, spiranes, alkylidene cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.

Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.

Simple chemical correlation of configurations with examples, quasiracemates.

Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (mono-, di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

Asymmetric induction: Cram's, Prelog's and Felkin-Ahn model; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

Molecular dissymmetry and chiroptical properties: Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. Eliel, E. L. *Stereochemistry of Carbon Compounds* Textbook Publishers (2003).
3. Finar, I. L. & Finar, A. L. *Organic Chemistry* Vol. 2, Addison-Wesley (1998).
4. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).
5. Lowry, T. H. & Richardson, K. S. *Mechanism and Theory in Organic Chemistry* Addison-Wesley Educational Publishers, Inc. (1981).
6. Nasipuri, D. N. *Stereochemistry of Organic Compounds: Principles & Applications* South Asia Books (1994).
7. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).
8. Singh S.P. and Om Prakash. *Reaction Mechanism* Laxmi Publications, Delhi (2017-18)
9. Kumar and Singh S.P. *Pericyclic Reactions*. Academic Press, London (2017-18)

Practical core course 2 (50 Marks/ 2 credits)

Organic Chemistry - 102

- i) Measurement of optical rotation values, calculation of *ee/de* ratios and determination of specific rotation
- ii) Chemical resolution of racemic mixtures of acids with chiral amines or amines with chiral acids
- iii) Analytical and preparative TLCs (mixtures containing three or more compounds, natural extracts and use of different developing agents)
- iv) Preparations involving stereochemical aspects (geometrical isomers and stereoisomers) and different reactive intermediates:
 - (a) Condensation reaction,
 - (b) Bromine addition,
 - (c) Carbene addition,
 - (d) Nucleophilic aromatic/aliphatic substitution reaction,
 - (e) Rearrangement reactions involving carbocations and carbanions
- v) Applications of UV and CD spectroscopy

Paper 103 - Physical Chemistry-I (Core course 3) (100 Marks/ 4 Credits)

Course A: Mathematical and quantum methods

Vectors: Differentiation and integration of vectors, scalar and vector fields, divergence & curl, Line integrals. Orthogonal curvilinear coordinates. Spherical polar coordinates.

Linear vector spaces, linear independence, basis vectors, inner product, Dirac bra-ket notation. Orthonormal sets. Completeness.

Linear operators, matrices as linear operators, geometrical operations. Properties of determinants. Special types of square matrices: diagonal, symmetric and anti-symmetric, Hermitian and anti-Hermitian, orthogonal matrices, unitary matrices, normal matrices. Eigenvectors and eigenvalues of Hermitian and unitary matrices. Cayley-Hamilton theorem, degenerate eigenvalues. Gram-Schmidt orthogonalization. Diagonalization of matrices. Change of basis and similarity transformation.

Limits and series. The extrema of a function and its critical points. Mean value theorem and L'Hôpital's rule, binomial expansion, tests of series convergence.

Fourier series, sine, cosine and exponential Fourier series. Fourier transform, Dirac delta function, Fourier sine and cosine transforms, applications of Fourier transforms.

Laplace transform and its inverse, Solution of initial value problems using Laplace transform.

Ordinary differential equations (ODE) and Partial differential equations: Linear independence. General solution of homogeneous equations. Power series solutions. Ordinary and singular points of an ODE. Legendre polynomials. General solution for integer l and second solution.

Special functions: Properties of Legendre polynomials. Orthogonality, Rodrigues' formula, Generalized Fourier-Legendre series, generating function, Recursion formulae, Associated Legendre polynomials. Hermite, Laguerre and associated Laguerre polynomials.

Ladder operators and recursion relations of Hermite polynomials, Generating functions, Rodrigues Representation. Derivation of H-atom (energy quantization), Virial theorem and its applications to harmonic oscillator and H-like atoms. Concept of spin, Stern-Gerlach experiment, algebra of two-electron spin systems and determinantal wavefunctions.

Course B: *Quantum Chemistry and Approximate Methods*

Postulates of Quantum mechanics, Linear and Hermitian operators, Turn-over rule, Commutation of operators and Uncertainty principle.

Some exactly soluble problems: Particle in a box (1-D, 2-D & 3-D) and ring. Concept of degeneracy and Jahn-Teller distortion.

Simple harmonic oscillator problem and its solution using series solution or factorization method. Calculation of various average values.

Angular momentum operators, Eigenvalues and eigen-functions, Rigid rotator and hydrogen atom Complete solution. Radial distributions.

Approximate methods: First order time-independent perturbation theory for non-degenerate states. Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

HMO method and its applications: π -Electron approximation, Huckel Molecular Orbital Theory of conjugated systems, Calculation of properties- Delocalization energy, electron density, bond order,

non-alternant hydrocarbons. Pairing theorem. Electronic and ESR spectra. Effect of substituents on spectra. Reactivity and electro-cyclic ring closures.

Chemical bonding: Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments and their equivalence limit. Configuration Interaction. Extension of MO theory to other systems- Homonuclear and heteronuclear diatomics, polyatomics, Walsh diagrams for dihydrides, linear and bent triatomics.

Ground and excited state of helium atom. Pauli's Exclusion principle, Many-electron atoms. Qualitative treatment of Hartree theory and Hartree-Fock SCF procedure through Slater Determinant wavefunctions. Illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

Recommended Texts:

1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
7. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).
8. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
9. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004)
10. Kreyszig, E., Advanced Engineering Mathematics, John Wiley & Sons, Inc. (2006)

Practical core course 3 (50 Marks/ 2 Credits)

Physical Chemistry - 104

Chemical Kinetics

1. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate by the *Initial Rate Method*. Study the reaction at two different temperatures and calculate the thermodynamic parameters.
2. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
3. Study the saponification of ethyl acetate with sodium hydroxide volumetrically.

Conductometry

1. (i) Determine the Cell Constant of the given conductivity cell at room temperature and study the equivalent conductance versus square root of concentration relationship of a strong electrolyte (KCl or NaCl) and weak electrolyte (acetic acid).
(ii) Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.

- (iii) Determine the equivalent conductance, degree of dissociation and dissociation constant (K_a) of acetic acid.
2. (i) Study the conductometric titration of hydrochloric acid with sodium carbonate and determine the concentration of sodium carbonate in a commercial sample of soda ash.
(ii) Study the conductometric titration of potassium sulphate solution vs. barium chloride solution
 3. Study the conductometric titration of
 - (i) Acetic acid vs. sodium hydroxide,
 - (ii) Acetic acid vs. ammonium hydroxide,
 - (iv) HCl vs. NaOH

Comment on the nature of the graphs.

4. Study the stepwise neutralization of a polybasic acid e.g. oxalic acid, citric acid, succinic acid by conductometric titration and explain the variation in the plots.

Potentiometry

1. Titrate hydrochloric acid and sodium hydroxide potentiometrically.
 - (ii) Determine the dissociation constant of acetic acid potentiometrically.
 - (iii) Titrate oxalic acid and sodium hydroxide potentiometrically.
2. Titrate a mixture of
 - (i) Strong and weak acids (Hydrochloric and acetic acids)
 - (ii) Weak acid (acetic acid) and dibasic acid (oxalic acid)
 - (iii) Strong acid (hydrochloric acid) and dibasic acid (oxalic acid) versus sodium hydroxide.
3. Titrate a solution of Mohr's salt against potassium permanganate potentiometrically. (ii).
Titrate a solution of Mohr's Salt and potassium dichromate potentiometrically.

Computational Methods

Familiarity with word processing, electronic spreadsheets, data processing, mathematical packages, chemical structure drawing and molecular modelling.

(Note. Any other experiment may be introduced during the year)

SEMESTER – II

Paper 201-Inorganic Chemistry-II (Core course 4) (100 Marks/ 4 Credits)

Course A: Group Theory and its Applications

Molecular symmetry: Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation.

Products of symmetry operations, equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups and classification.

Symmetry: Optical activity and dipole moment.

Representation of groups, reducible and irreducible representations. The Great Orthogonality theorem, character tables, position vector and base vector as basis for representation.

Wavefunctions as bases for irreducible representations (*p*- and *d*-orbitals). Direct product.

Spectral transition probability, vibronic coupling, non-centrosymmetric complexes, polarization of allowed transitions.

Application of Group Theory in Infrared and Raman Spectroscopy.

SALCs, projection operators, illustrative examples.

Hybridization and its applications, Hybrid orbitals as Linear Combinations of Atomic Orbitals. Selected examples. MO diagram using Group Theory.

Symmetry and chemical reactions.

Course B: Chemistry of *d*- and *f*-block elements:

Term-symbols, Russell-Saunders states, Crystal field theory and splitting in O_h , T_d , D_{4h} and C_{4v} systems, Orgel and Tanabe-Sugano diagrams, determination of Dq and Racah parameters, oxidation states and electronic absorption spectra of complex ions. Spectrochemical series and effects of covalency. Nephelauxetic series, magnetic properties of transition metal complexes and lanthanides, metal-metal bonds, cluster compounds of *d*-block elements, poly-oxo metallates of Ru, Os, Mo. Structure and bonding in complexes containing π -acceptor ligands. Relativistic effects affecting the properties of heavier transition elements.

Recommended Texts:

1. Jaffe, H. H. & Orchin, M. *Symmetry in Chemistry* Dover Publications (2002).
2. Cotton, F. A. *Chemical Applications of Group Theory* Wiley Interscience: N.Y (1990).
3. Hatfield, W. E. & Parker, W. E. *Symmetry in Chemical Bonding & Structure* C. E. Merrill Publishing Co.: USA (1974).
4. Bishop, D. M. *Group Theory and Chemistry*, Clarendon Press: Oxford, U.K. (1973).
5. Shriver, D. F., Atkins, P. W. & Langford, C. H. *Inorganic Chemistry*, 2nd Ed., Oxford Univ. Press (1998).
6. Purcell, K. F. & Kotz, J. C. *Inorganic Chemistry*, W. B. Saunders and Co.: N. Y. (1985).
7. Wulfsberg, G. *Inorganic Chemistry* Univ. Science books: Viva Books: New Delhi (2000)
8. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes* Chapman and Hall: U.K. (1973).
9. Drago, R. S. *Physical Methods in Chemistry* W. B. Saunders Co.: U.K. (1982).

Practical Core Course 4 (50 Marks/ 2 Credits)

Inorganic Chemistry - 201

1. Qualitative analysis of mixtures of salts including rare element salts (soluble and insoluble) containing eight radicals including interfering ions.
2. Determination of some metal ions, such as iron, nickel, etc. by colorimetric method.
3. Any other experiments done in the class during the semester.

Paper 202- Organic Chemistry-II (Core course 5) (100 Marks/ 4 Credits)

Course A: Spectroscopy of Organic Compounds

PMR: Natural abundance of ^{13}C , ^{19}F and ^{31}P nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, spin-spin coupling, splitting theory, magnitude of coupling constant; Simple, virtual and complex spin-spin coupling; Chemical and magnetic equivalence, proton exchange, factors affecting the coupling - First and non-first order spectra; Simplification of complex spectra (solvent effect, field effect, double

resonance and lanthanide shift reagents) and NOE experiments (NOESY, HOESY, ROESY, etc.). Applications of PMR in structural elucidation of simple and complex compounds.

CMR: Resolution and multiplicity of ^{13}C NMR, ^1H -decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and INEPT experiments; Introduction to 2D-NMR; COSY, HMQC and HETEROR spectra.

MASS: Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms-singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M^+ ion peak; Ionization methods (EI, CI, FAB, ESI, APCI and MALDI), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α -, β -, allylic and benzylic cleavage; McLafferty rearrangement, ortho effect etc.

Structure elucidation of organic compounds using IR, NMR and Mass Spectra

Course B: Reagents and Methods in Organic Synthesis

Organosilicone Compounds: Preparation and applications in organic synthesis.

Applications of Pd(0) and Pd(II) complexes in organic synthesis: Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling.

Preparation and applications of lithium organocuprates.

Reductions: Stereochemistry, stereoselection and mechanism of catalytic hydrogenation and metal-liquid ammonia reductions.

Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithium aluminium hydride and alkoxy substituted LAH reducing agents, DIBAL; Applications of hydroboration (reductions, oxidations and carbonylations): diborane, diisoamylborane, hexylborane, 9-BBN, isopinocampheyl and diisopinocampheyl borane.

Homogeneous hydrogenations: Mechanisms and applications using Rh, Ru and other metal complexes.

Oxidations: Scope of the following oxidizing reagents with relevant applications and mechanisms: DDQ, SeO_2 , $\text{Ti}(\text{NO}_3)_3$, Sharpless Asymmetric epoxidation, Asymmetric hydroxylation and aminohydroxylation.

Recommended Texts:

1. Carruthers, W. *Modern Methods of Organic Synthesis* Cambridge University Press (1996).
2. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
3. Kemp, W. *Organic Spectroscopy* 3rd Ed., W. H. Freeman & Co. (1991).
4. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. *Spectroscopic Identification of Organic Compounds* John Wiley & Sons (1981).
5. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. *Introduction to Spectroscopy* Cengage Learning (2014).
6. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).
7. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007

Practical Core Course 5 (50 Marks/ 2 credits)

Organic Chemistry-202

A. Organic Synthesis

- i) Protection and deprotection reactions of carboxylic acids, amines, alcohols, 1,2-diols, aldehydes/ketones, etc.
- ii) Oxidation reactions of alcohols, aldehydes, etc.
- iii) Reduction reactions of aldehydes/ ketones, carboxylic acids, carbon-carbon multiple bonds, nitro compounds
- iv) Metals/ metal salts catalyzed coupling reactions
- v) Diels-Alder reactions
- vi) Bromination reactions involving allylic/ benzylic bromination and aromatic substitution reactions
- vii) Diazotisation reactions for substitutions and couplings
- viii) Condensation reactions
- ix) Esterification, transesterification and hydrolysis reactions
- x) Preparation of phenoxyacetic acids and 2,4-D (2, 4-dichlorophenoxyacetic acid)

B. Application of IR spectra and introduction to NMR spectra of simple compounds

Paper 203- Physical Chemistry-II (Core course 6) (100 Marks/ 4 Credits)

Course A: Statistical Mechanic and Thermodynamics

Fundamentals: Idea of microstates and macrostates. Concept of distributions- Binomial & multi-nomial distributions for non-degenerate and degenerate systems, Thermodynamic probability and most probable distribution. Canonical and other ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.

Einstein theory and Debye theory of heat capacities of monatomic solids.

Third law of thermodynamics, Residual entropy.

Course B: Macromolecules, Electrochemistry and Kinetics

Macromolecules: Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. 1-D random walk model in detail, Average end-to-end distance.

Electrochemistry: Solutions: Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination. Derivation of the Debye-Hückel theory of activity coefficients (both point ion size and finite ion size models). Excess functions.

Theories of reaction rates: Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

Solution kinetics: Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Recommended Texts:

1. McQuarrie, D. A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
2. Bagchi B. *Statistical Mechanics for Chemistry and Material Science*, CRC Press (2018).
3. L. D. Landau and E. M. Lifshitz, *Statistical Mechanics, Part I*, Butterworth-Heinemann, 3rd ed. (2005).
4. J. M. Bockris and A. K. N. Reddy, *Modern Electrochemistry 1 (Ionics)*, Springer (2006).
5. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
6. Billmeyer, F. W. *Textbook of Polymer Science* 3rd Ed. Wiley-Interscience: New York (1984).
7. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
8. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).

Practical Core Course 6 (50 Marks/ 2 Credits)

Physical Chemistry (50 marks) (Core practical 6)

CHEMICAL KINETICS

1. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the *Initial Rate Method*.
2. Study the kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.

CONDUCTOMETRY

1. Study the conductometric titration of a mixture of a strong and weak acid.
2. Titrate a moderately strong acid (salicylic/ mandelic acid) by the
(a) salt-line method
(b) double alkali method.
3. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid with sodium hydroxide.
4. Titrate a tribasic acid (phosphoric acid) against NaOH and Ba(OH)₂ conductometrically.
5. Titrate magnesium sulphate against BaCl₂ and its reverse titration
6. Estimate the concentration of each component of a mixture of AgNO₃ and HNO₃ by conductometric titration against NaOH.
7. Determine the degree of hydrolysis of aniline hydrochloride.

POTENTIOMETRY

1. Determine the solubility and solubility product of an insoluble salt, AgX (X=Cl, Br or I) potentiometrically.

2. Determine the mean activity coefficient (γ_{\pm}) of 0.01 M hydrochloric acid solution.
3. Titrate phosphoric acid potentiometrically against sodium hydroxide.
4. Find the composition of the zinc ferrocyanide complex by potentiometric titration.
5. Titrate potentiometrically solutions of
 - (a) KCl/ KBr/ KI;
 - (b) mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
6. Titrate Fe^{2+} with Ce^{4+} potentiometrically.
7. Determine zinc in the presence of calcium by potentiometric titration.
8. Verify the Debye-Hückel theory through the solubility of ionic salts.

(Note: Depending on availability of time, some experiments may be added/deleted during the semester.)

M.Sc. Part II

SEMESTER – III

Paper 301- Inorganic Chemistry-III (Core course 7) (100 Marks/ 4 Credits)

Course A: Inorganic Reaction Mechanisms

Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, factors affecting the reactivity of square planar complexes, Swain-Scott equation, Trans effect and its application to synthesis of complexes.

Molecular rearrangement processes: Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reluctant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

Course B: Catalysis and Bio-inorganic Chemistry

Transition metal ion catalysts for organic transformations and their application in hydrogenation (using symmetric and chiral organometallic catalysts), isomerization, olefin oxidation, carbonylation and polymerization reactions. Role of metal ions in biological systems. Toxic metal ions and their detoxification, chelation therapy/chelating agents in medicine. Recent advances in cancer chemotherapy using chelates. Biological nitrogen fixation. Natural and synthetic oxygen carriers. Na-K, ATPase or sodium pump. Futuristic aspects of organo transition metal complexes as catalysts and in bio-inorganic chemistry.

Recommended Texts:

1. Drago, Russell S. *Physical Methods for Chemists 2ed.* East West Press Pvt. Ltd. (2016).
2. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes.* Dover Publications; 2008 edition (2008).
3. Roberts, A. P. *Polyoxometalates: Properties, Structure and Synthesis,* Nova Science Publishers, Incorporated (2016).
4. Kettle. S. F. A. *Physical Inorganic Chemistry: A Coordination Chemistry Approach,* Springer, Berlin, Heidelberg (1996).
5. Hughes, M. N. *The Inorganic Chemistry of Biological Processes,* 2nd Ed., Wiley (1981).
6. Masters, C. *Homogeneous Transition Metal Catalysis* Chapman & Hall (1981).
7. Purcell, K. F. & Kotz, J. C. *Inorganic Chemistry,* Cengage Learning India private Ltd., New Delhi (2010)
8. Asperger, S. *Chemical Kinetics and Inorganic Reaction Mechanisms,* Springer-US, New York (2003)

Paper 302-Organic Chemistry-II (Core course 8) (100 Marks/ 4 Credits)

Course A: Photochemistry & Pericyclic Reactions

Photophysical processes: Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects, Stern-Volmer plot, delayed fluorescence, etc.

Photochemistry of alkenes: cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes; dimerizations.

Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic); α,β -unsaturated ketones; β,γ -unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno–Buchi reactions; photoreductions.

Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar and prismanes in isomerization. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loeffler-Freytag reaction.

Pericyclic reactions: Electrocyclic, cycloaddition, sigmatropic and chelotropic reactions; General Orbital Symmetry rules, Frontier Orbital approach, PMO approach, Correlation diagrams for different systems, Hückel–Möbius approach, General pericyclic selection rule and its applications, 1,3-dipolar additions, Ene reaction.

Course B: Medicinal Chemistry

Introduction to the history of medicinal chemistry.

General mechanism of drug action on lipids, carbohydrates, proteins and nucleic acids, Drug metabolism and inactivation. Receptor structure and sites.

Drug discovery, development, design and delivery systems.

General introduction to antibiotics, Mechanism of action of lactam antibiotics, non-lactam antibiotics and quinilones; antiviral and anti-AIDS drugs.

Neurotransmitters, classes of neurotransmitters, Drugs affecting collingeric and adrenergic mechanisms.

Anti-histamines, anti-inflammatory, anti-analgesics, anticancer and anti-hypertensive

drugs. New developments, e.g. gene therapy, anti-sense & anti-gene strategies and drug resistance.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. Horspool, W. M. *Aspects of Organic Photochemistry* Academic Press (1976).
3. Lowry, T. H. & Richardson, K. S. *Mechanism and Theory in Organic Chemistry* Addison-Wesley Educational Publishers, Inc. (1981).
4. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).
5. Fleming, I., *Pericyclic Reactions*, Oxford Science Publications (1998).
6. Marchand, A. P. & Lehr, R. E. *Pericyclic Reactions* Academic Press (1977).
7. Gringauz, A. *Introduction to Medicinal Chemistry: How Drugs Act and Why?* John Wiley & Sons (1997).
8. Patrick, G. L. *Introduction to Medicinal Chemistry* Oxford University Press (2001).
9. Lemke, T. L. & William, D. A., *Foye's Principles of Medicinal Chemistry*, 5th Ed., USA, (2002)

Paper 303- Physical Chemistry-III (Core course 9) (100 Marks/ 4 Credits)

Molecular Structure: Spectroscopic and Diffraction Methods

Course A: Spectroscopic methods

Characterization of electromagnetic radiation. Born-Oppenheimer approximation. Heisenberg's Uncertainty Principle. Basic elements of spectroscopy. Time dependent perturbation. Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Molecular spectroscopy: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and / or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First and second order Stark effect.

Vibrational spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones. Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect. Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules. Overtones and combination bands.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and vibrational Raman spectroscopy. Selection rules. Rule of Mutual Exclusion. Polarization of Raman lines.

Course B: Diffraction & Resonance Methods

Diffraction Methods. Atomic scattering factors. Scattering by a small crystal. Direct and reciprocal lattice. Miller indices. Bragg's law and Laue's equations. Structure factors. Systematic absences for different types of unit cells (primitive, face-centred, body-centred, side-centred) and application to some common metal and metal salt structures (rock salt, zinc blende, etc.). Space groups. Glide planes and screw axes. Structure determination for organic crystals like naphthalene. Fourier series, Patterson's functions. Heavy atom method. Comparison of X-ray method with electron and neutron diffraction methods. Band structure of solids.

NMR spectroscopy: Larmor precession. Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation. Quantum mechanical treatment of the AB system. Selection rules and relative intensities of lines.

Electron Spin Resonance spectroscopy: Basic principles. Relaxation and line-widths. Zero-field splitting and Kramer's degeneracy. g -factor for paramagnetic ions. g -factor for organic radicals. Factors affecting the g -factor. Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and McConnell relationship. Fine splitting in triplet spectra. Applications of ESR spectroscopy - Structure determination, Interpretation of ESR spectra of simple organic radicals like benzene radical anion, naphthalene radical anion, toluene and *o*-, *m*- and *p*-xylene radical ions from HMO theory. Study of unstable

paramagnetic species, Kinetic studies of electron transfer reactions, Spin-labelling studies of biomolecules.

NQR spectroscopy: Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting. Applications.

Principles of Mössbauer spectroscopy: Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Recommended Texts:

1. Hollas. J. M. *Modern Spectroscopy* 4th Ed., John Wiley & Sons (2004).
2. Satyanarayana, D. N. *Handbook of Molecular Spectroscopy: From radio waves to gamma rays*, I.K. International Publishing House, New Delhi (2015).
3. Kakkar, R., *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).
4. Brand, J. C. D. & Speakman, J. C. *Molecular Structure: The Physical Approach* 2nd Ed., Edward Arnold: London (1975).
5. Chang, R. *Basic Principles of Spectroscopy* McGraw-Hill, New York, N.Y. (1970).
6. Moore, W. J. *Physical Chemistry* 4th Ed. Prentice-Hall (1972).
7. Warren, B. E. *X-Ray Diffraction* Dover Publications (1990).
8. Bacon, G. E. *Fifty Years of Neutron Diffraction* Hilger (1987).

Paper 3101-Inorganic Chemistry (Special-II/ Open Elective 1)

Course A: Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds

Chemistry of inorganic rings, cages and metal cluster compounds, borazines, phosphazenes, polyhedral boranes, carboranes, metalloboranes and metallocarboranes.

Silicates and aluminosilicates

Classifications, structure, properties and applications of naturally occurring silicates and aluminosilicates.

Syntheses of pillared clays, and zeolites.

Characterization of clays, pillared clays and zeolites from measurement of surface area, surface activity pore size, distribution and interlayer spacing.

Application of clays, pillared clays and zeolites with emphasis of catalyses.

Course B: Introduction to the Solution of Multielectron Problems

Introduction to the solution of multielectron problems, the central field approximation, angular momenta, step up and step down operators and their use in atomic spectra. Lande's interval rule. Evaluation of energy matrices using Slater's method. Wave functions forming basis for irreducible representations, direct product. Spherical harmonics and their linear combinations. Operator equivalent technique.

The octahedral potential, contribution of spherical harmonics to the octahedral potential V_{xyz} . Single

electron in a cubic field, quantitative basis (r, θ, ϕ) for the splitting of d orbitals to e_g and t_{2g} in terms of D_q , multielectron systems - the weak and strong field cases. Generation of a secular determinant for 3F term (d^2) in weak field. Bethe's method of descending symmetry. Non octahedral fields, tetrahedral (including contribution of odd harmonics), trigonal and tetragonal (including D_s & D_t parameters). Spin orbit coupling and its magnitude in comparison to crystal field. Splitting of e_g and t_{2g} orbitals due to spin orbit coupling, for the

d^1 and d^9 case. The use of double groups D_4' and O' . Effect of spin orbit coupling on A, E and T terms in octahedral fields.

Recommended Texts:

1. B.N. Figgis and M.A. Hitchman, Ligand Field Theory and its Applications, Wiley (2010).
2. Sels, B.F. & Kustov, L.M. Zeolites and Zeolite-like materials 1st Edition, Elsevier (2016).
3. Wells, A.F. Structural Inorganic Chemistry, 5th Edition, Oxford University Press, Oxford (1984).
4. Adams, D.M. Inorganic Solids. An Introduction to Concepts in Solid-State Structural Chemistry, John Wiley & Sons, London (1974).
5. Liebau, F. Structural Chemistry of Silicates: Structure, Bonding, and Classification, Springer-Verlag Berlin Heidelberg (1985).

Paper 3102-Inorganic Chemistry (Special III/ Open Elective I)

Introduction to Nanochemistry

Course A: Properties of Nanomaterials

Introduction: Properties of materials & nanomaterials, role of size and shape in nanomaterials.

Electronic Properties: Classification of materials: Metal, Semiconductor, Insulator, Band structures, Brillouin zones, Mobility, Resistivity.

Magnetic Properties: Superparamagnetism, blocking. Important properties in relation to nanomagnetism.

Optical Properties: Photoconductivity, Optical absorption & transmission, Photoluminescence, Fluorescence, Phosphorescence, Electroluminescence.

Thermal Properties and Mechanical Properties;

Course B: Synthesis and Characterization of Nanomaterials

Chemical Methods: Metal nanocrystals by reduction, Solvothermal synthesis, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, Post-synthetic size-selective processing. Sol-gel, Micelles and microemulsions.

Biological Methods of Synthesis: Use of bacteria, fungi, Actinomycetes for nanoparticles synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Mechanism of formation; Viruses as components for the formation of nanostructured materials; Synthesis process and application, Role of plants in nanoparticle synthesis.

Characterization Techniques: X-ray diffraction, Scanning Probe Microscopy, SEM, TEM, Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-VIS-IR Spectrophotometers.

Recommended Texts:

1. Dupas, C., Houdy, P. & Lahmani, M. *Nanoscience: Nanotechnology and Nanophysics*, Springer (2004)
2. Klabunde, K. J., Ed. *Nanoscale Materials in Chemistry*, Wiley Interscience (2001)
3. Kulkarni, S. K. *Nanotechnology: Principles and Practices*, Capitol Publishing Company (2007)

4. Wilson, M., Kannangara, K., Smith, G., Simmons, M. & Raguse, B. *Nanotechnology: Basic Science and Emerging Technologies*, Overseas Press (2005).
5. Poole Jr., C. P. & Ovens, F. J. *Introduction to Nanotechnology*, Wiley Interscience (2003)
6. Edelstein, A.S. & Cammarata, R. C., Ed. *Nanomaterials: Synthesis, Properties and Applications*, Institute of Physics Publishing (1996)
7. Rao, C.N.R., Müller & Cheetham, A.K., Eds. *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004)
8. Edelstein, A.S. & Cammarata, R.C., Ed. *Nanomaterials: Synthesis, properties and Applications*, Institute of Physics Publishing (1996).

Paper 3201- Organic Chemistry (Special-II/ Open Elective-1) (100 Marks/ 4 Credits)

Chemistry of Life Processes and Bioactive Compounds

Course A: Chemistry of Life Processes

Introduction to metabolic processes: Catabolism and anabolism, ATP- currency of biological energy, energy rich and energy poor phosphates, role of NADH, NADPH, FADH₂, TPP, coenzyme A, lipoic acid and biotin.

Carbohydrate metabolism: Glycolysis, fate of pyruvate under anaerobic conditions, citric acid cycle, oxidative phosphorylation (electron transport system), gluconeogenesis, C₄ pathway, pentose phosphate pathway and photosynthesis.

Fatty acid metabolism: Even chain and odd chain (saturated and unsaturated) fatty acids, ketone bodies, fatty acid anabolism, calorific values of food.

Protein metabolism and disorders: Degradation of amino acids (C₃, C₄, C₅ family), urea cycle, uric acid and ammonia formation.

Enzymes: Enzyme active sites, allosteric sites and mechanisms of their actions, e.g. chymotrypsin, carboxypeptidase, lipases, etc.

Nucleic acids: Chemical and enzymatic hydrolysis, purine metabolism, structure and functions of DNA, RNA (m-RNA, t-RNA, r-RNA), genetic code (origin, Wobble hypothesis and other important features), genetic errors.

Course B: Bioactive Compounds

Vitamins: Classification, occurrence, chemistry of Vitamins A, C and E, structure elucidation and synthesis, deficiency syndromes, etc.

Insect hormones: Introduction to BH, JH and MH, chemistry of JH, structure elucidation and synthesis, structural analogs, biosynthesis; JH mimics– some structures; chemistry of Juvabione.

Precocenes: Chemistry of Precocene I and II.

Antifeedants: Different classes of antifeedants; role of azadirachtin in IPM.

Pyrethroids: Introduction; structure elucidation and synthesis of pyrethroids, namely pyrethrins, cinerins and jasmoline; Synthetic pyrethroids: Structure–activity relationships; synthesis of various synthetic pyrethroids.

Insect pheromones: Semiochemicals, pheromones, primers and releasers, different classes of pheromones, synthesis of different pheromones; advantages of pheromones over conventional pesticides.

Hormones: General study of hormones including classification, mechanism of action of water soluble and fat soluble hormones, secondary messengers, negative feedback mechanism; Antifertility agents.

Recommended Texts:

1. Stryer, L. *Biochemistry* 4th Ed., W. H. Freeman & Co. (1995).
2. Zubay, S. *Biochemistry* Addison-Wesley (1983).
3. Litwak, G. *Vitamins and Hormones*, Academic Press, (2005)
4. Dugas, H. & Penney, C. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action* Springer-Verlag (1989).

Paper 3202- Organic Chemistry (Special-III/ Open Elective-1) (100 Marks/ 4 Credits)

Course A: Polymer Chemistry and Processing

Introduction: Polymers and their classification.

Synthesis of Polymers: Chemistry of radical, anionic and cationic polymerization; Ziegler–Natta catalysts; Polycondensation and ring opening polymerization.

Methods of polymerization: Bulk, solution, suspension and emulsion polymerizations.

Geometry of the polymers: Homopolymers; copolymers; branched-polymers; crosslinked polymers; random, alternating, block and graft copolymers; star polymers and dendrimers; tacticity of polymers.

Characterization of polymers: Molecular weight determination of polymers; thermal properties of polymers; Glass transition temperature; plasticizers.

Polymer Processing: Injection moulding, compression moulding, blow moulding, Extrusion compounding, elastomer properties, vulcanization, reinforcement, fillers, plasticisers and other additives.

Course B: Role of Catalysis in Chemical Synthesis

The art of catalysis, Thermodynamic data and catalyst designing, Metal catalyzed organic reactions, characteristics of transition metals which make them suitable as catalysts; Homogeneous and heterogeneous catalysts and their characterization.

Catalyst and molecular activation, Catalytic reaction and the 16 electron rule, Catalysts for fine chemical synthesis, transition metal ion catalysts for organic transformations and their applications in epoxidation of alkenes, isomerization of unsaturated molecules, Alkene Metathesis, Oligomerisation and polymerization (Ziegler Natta polymerization), olefin oxidation (Wacker Process), Hydroformylation (oxoreaction), Fischer-Tropsch Reaction, The water- Gas Shift Reaction, Monsanto Acetic Acid Process, Reppe Carbonylation, Hydrocyanation, activation of C-H bond, Green Chemistry and Catalysis, Computer applications in catalysis research.

Recommended Texts:

1. Billmeyer Jr., F. W. *Textbook of Polymer Science* 3rd Ed. Wiley-Blackwell (1984)
2. Odian, G. *Principles of Polymerization* 4th Ed. Wiley (2004)
3. Hodge, P. & Sherrington, D.C. *Polymer-supported Reactions in Organic Synthesis* John Wiley & Sons (1980)
4. Collman J.P. & Hegedus Louis S., *Principles and Application of Organotransition Metal Chemistry*, University Science Books (1980).
5. Elschenbroich C. & Salzer A. *Organometallics: A Concise Introduction* VCH (1989).
6. Roberts, S.M. & Poignant, G., Eds. *Catalysis for Fine Chemical Synthesis*, Volume 1-5, John Wiley & Sons (2002)
7. Sheldon, R.A., Isabel, A. & Hanefeld U., *Green Chemistry and Catalysis*, Wiley-VCH (2007).

Paper 3301- Physical Chemistry (Special-I/ Open Elective 1) (100 Marks/ 4 Credits)

Irreversible Thermodynamics, Transport Phenomena, Surface Phenomena & Fast Reactions

Course A: Irreversible thermodynamics and transport phenomena

Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for non-equilibrium states, Phenomenological laws- Linear laws, Gibbs equation, Onsager's reciprocal relations, Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena. Some important applications.

Transport phenomena: Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path, relation between thermal conductivity/viscosity and mean free path of a perfect gas, Einstein relation, Nernst-Einstein equation, Stokes-Einstein equation, Einstein-Smoluchowski equation.

Course B: Interfacial Phenomenon and Fast reaction

Surface phenomena: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature, Factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, surface films (electrokinetic phenomena), catalytic activity at surfaces. Electrode/electrolyte interface; electrical double layer, electrode kinetics, Nernst equation. Application of PES, ESCA and Auger spectroscopy to the study of surfaces.

Fast reactions: Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method. Kinetics of solid-state reactions.

Recommended Texts:

1. Rastogi, R. P., Introduction to Non-equilibrium Physical Chemistry, Elsevier B.V. (2008)
2. Kalidas, C. & Sangaranarayanan, M.V. Non-Equilibrium Thermodynamics: Principles & Applications, Macmillan India Ltd. (2002).
3. Katchalsky, A. & Curran, P. F. *Non Equilibrium Thermodynamics in Biophysics* Harvard University Press: Cambridge (1965).
4. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).

5. Thomas, J. M. & Thomas, M. J. *Principles and Practice of Heterogeneous Catalysis* John Wiley & Sons (1996).
6. Chorkendorff, Ib. & Niemantsverdriet, J. W. *Concepts of Modern Catalysis and Kinetics* Wiley-VCH (2003).
7. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
8. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
9. Shaw, D. J. *Introduction to Colloid and Surface Chemistry* 2nd Ed. Butterworths (1970).
10. Adamson, A. W. & Gast, A. P. *Physical Chemistry of Surfaces* 6th Ed. Wiley Interscience.(1997)

SEMESTER - III

PRACTICALS SYLLABUS

Paper 3103: Practical Inorganic Chemistry - I (Elective practical 1) (200 Marks/ 8 credits)*

Part – A: Synthesis and Analysis

I. Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR spectroscopy, magnetic susceptibility etc. Selection can be made from the following or any other from the existing literature.

- (i) Metal acetylacetonates
- (ii) *Cis* and *trans* isomers of $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$
- (iii) Ion-exchange separation of oxidation states of vanadium.
- (iv) Preparation of Ferrocene.
- (v) Preparation of triphenyl phosphene Ph_3P , and its transition metal complexes.
- (vi) Determination of Cr(III) complexes.
 $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_3 \cdot 3\text{H}_2\text{O}$; $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl} \cdot 2\text{H}_2\text{O}$; $[\text{Cr}(\text{en})_3]\text{Cl}_3$; $\text{Cr}(\text{acac})_3$.
- (vii) Tin(IV) iodide, Tin(IV) chloride, Tin(II) iodide.
- (viii) (*N,N*)-bis(salicylaldehyde)ethylenediamine Salen H₂; and its cobalt complex $[\text{Co}(\text{Salen})]$.
- (ix) Reaction of Cr(III) with multidentate ligands, a kinetics experiment.
- (x) Vanadyl acetylacetonate.
- (xi) Mixed valence dinuclear complex of Manganese(III,IV).
- (x) Other new novel synthesis reported in literature from time to time
- (xi) Any other experiments done in the class during the current academic semester.

Part – B: Instrumental based Analysis: Any three/four techniques covered in the semester out of the following syllabus:

- (1) Instrumental methods of analysis utilizing flame photometer, atomic absorption spectrophotometer, pH-meter, potentiometer, turbidimeter, electrochemical methods, separation of mixtures of metal ions by ion exchange chromatography.
- (2) Synthesis and thermal analysis of group II metal oxalate hydrates.

(3) Any other experiments done in the class during the current academic semester.

Paper 3203: Practical Organic Chemistry - I (Elective practical 1) (200 Marks/ 8 Credits)*

Part A

1. Semi-micro qualitative analysis of single/polyfunctional compounds including derivatization
2. Application of spectral data (IR, UV, NMR and mass) for structural elucidation
3. Isolation of natural products:
 - i) Isolation of caffeine from tea leaves
 - ii) Isolation of piperene from black pepper
 - iii) Isolation of β -carotene from carrots
 - iv) Isolation of lycopene from tomatoes
 - v) Isolation of limonene from lemon peel
 - vi) Isolation of Eugenol from cloves
 - vii) Isolation of Cystine from human hair
 - viii) Isolation of DNA from Onion/ Strawberries

Part B

4. Quantitative analysis:
 - i) Estimation of glucose by chemical methods
 - ii) Estimation of amino acids by chemical methods
 - iii) Estimation of nitro group in organic compounds
 - iv) Estimation of iodine number by V_{ij}'s solution
 - v) Estimation of protein, caffeine and glucose by UV/VIS spectra (quantitative analysis also)
 - vi) Estimation of ascorbic acid by chemical/UV methods
 - vii) And other possible estimations
5. Advanced organic synthesis:

Multistage synthesis including photochemical methods; representative examples:

 - i) Benzophenone \rightarrow benzopinacol \rightarrow benzopinacolone
 - ii) Benzoin \rightarrow benzil \rightarrow benzilic acid
 - iii) Benzaldehyde \rightarrow chalcone \rightarrow chalcone epoxide
 - iv) Chalcone \rightarrow chalcone dibromide \rightarrow α -bromo-chalcone
 - v) Cyclohexanone \rightarrow cyclohexanone oxime \rightarrow caprolactone
 - vi) And other suitable multi-step synthesis

Paper 3302: Practical Physical Chemistry – I (Elective practical 1) (200 Marks/ 8 Credits)*

Set A

SPECTROPHOTOMETRY

1. Study the visible region absorbance spectra of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$.
2. Study the influence of pH on the spectrum of potassium dichromate solution.
3. Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture by the MLRA method.
4. Study the effect of structure on the UV spectra of organic compounds.
5. Determine the solvent cut-off wavelengths for the given solvents.
6. Study the effect of solvent on the UV spectra of organic compounds (propanone).
7. Study the spectra of mesityl oxide/ benzophenone in different solvents and classify

the observed transitions in terms of $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ transitions. Discuss the shift in transitions relative to those in acetone.

8. Determine the dissociation constant of phenolphthalein spectrophotometrically.

Set B

COLOURIMETRY

1. Verify Lambert-Beer's law, and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration *colourimetrically*.
2. Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture.
3. Study the kinetics of iodination of propanone *colourimetrically* in acidic medium.
4. Find the order and the energy of activation of the decomposition of the violet coloured Ce(IV) oxidation product of *N*-phenylanthranilic acid using a *colourimeter* (*J. Chem. Ed.*, 327 (1976)).
5. Determine the amount of iron present in a sample using 1,10-phenanthroline.
6. Determine the dissociation constant of an indicator (phenolphthalein) *colourimetrically*.
7. Study the kinetics of the reaction of phenolphthalein with sodium hydroxide.
8. Study the kinetics of the reaction of crystal violet with sodium hydroxide.

Set C

COMPUTATIONAL TECHNIQUES

- I. Use of spreadsheets and mathematical packages in data analysis and solving problems in chemistry (e.g. potentiometric titrations, kinetics, regression, and solving simultaneous equations).
- II. Elements of the BASIC language, including strings and graphics.

Set D

CONDUCTOMETRY

1. Determine the critical micelle concentration of a surfactant (sodium lauryl sulphate) by the conductivity method.
2. Study the effect of dielectric constant (ϵ) on the nature of the conductometric titration between maleic acid and sodium methoxide using different combinations of methanol and hexane as solvents.
3. Determine the velocity constant for the saponification of ethyl acetate conductometrically.

VISCOMETRY

4. Determine the molecular weight of a given macromolecule (PVP) by the viscosity method.
5. Determine the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.

NEPHELOMETRY

6. Estimate the concentration of sulphate ions in solution and in a sample of tap water by precipitation with barium chloride.
7. Estimate chloride ions in a given solution/ water from various sources.

ULTRASONIC STUDIES

8. Find the ultrasonic sound velocity (u) and isentropic compressibility (K_s) for the following pure solvents as a function of temperature: Water, DMF, DMSO, Methanol, Ethanol, 1-propanol
9. Measure the ultrasonic sound velocities as a function of temperature over the whole composition range for the following binary mixtures: DMF/Water, DMSO/Water, DMF/Methanol, DMF/Ethanol, DMF/1-propanol, DMSO/Methanol, DMSO/Ethanol, DMSO/1-propanol, Methanol/Water, Ethanol/Water, 1-propanol/Water.

SET E

NANOSCIENCE

1. Synthesize metallic (gold, silver, etc.) nanoparticles by reducing the corresponding salts with tea extract and characterize using UV-Vis spectroscopy. Estimate the size of these nanoparticles using the quantum mechanical equation for the particle in a 3D cubic box. Use the statistical mechanics method to determine the average occupancy level at room temperature.
2. Synthesize silver nanoparticles using a green approach and show its catalytic activity in reduction of methyl orange and rhodamine. Also study the kinetics of this process.
3. Estimate the optical energy gap of CdS nanoparticles doped with MnS in microemulsion media.
4. Study the effect of water/oil ratio in AOT isooctane based microemulsion on the particle size and bandgap of CdS nanoparticles.

SET F

CHRONOAMPEROMETRY, CYCLIC VOLTAMMETRY, EIS DATA ANALYSIS

1. (a) Verify the Cottrell equation using potential step chronoamperometry.
(b) The surface area of an electrode is determined via a chronoamperometric measurement.
(c) Determine the diffusion coefficient of the ion $[\text{Fe}(\text{CN})_6]^{3-}$
2. Record the effect of supporting electrolyte concentration on the Cottrell response.
3. Record the effect of solution viscosity on the Cottrell response and determine true area of a Pt electrode.
4. Verify the Randles-Sevcik equation for cyclic voltammetry. Use a reversible system (10 mM mixture of $\text{K}_3[\text{Fe}(\text{CN})_6]$ and $\text{K}_4[\text{Fe}(\text{CN})_6]$ in 2 M KCl). Identify the peak current and peak potential at different scan rates. Verify the reversibility of $\text{Fe}^{2+}/\text{Fe}^{3+}$ system by using ratio cathodic and anodic of peak currents.
5. Find quantities such as
 - i) Formal potential (E^0), (ii) Number of electrons transferred, (iii) Diffusion coefficient (D), (iv) Area (A) and concentration (C) by using CV.
6. Determine the best fit model and extract electrochemical system parameters from the given impedance data using **equivalent circuit models**, viz. Resistor capacitor, Randles, Warburg, CPE, CPE with diffusion, etc.

(Note: Depending on availability of time, some experiments may be added/deleted during the semester or interchanged with experiments from IV semester.)

SEMESTER IV

Inorganic Chemistry Special Papers

Paper 4101- Inorganic Chemistry (Special-III) (Elective paper 1) (100 Marks/ 4 Credits)

Spectral Techniques in Inorganic Chemistry

Course-A: Vibrational Spectroscopy, Mössbauer Spectroscopy, Magnetism & Mass Spectrometry

Vibrational spectroscopy: Vibrational motion and energies, number of vibrational modes, anharmonicity, absorption in infrared, FT spectrometers, cell systems, effects of phase on spectra, vibrational spectra and symmetry, selection rules, symmetry of an entire set of normal vibrations, F and G matrix. Raman spectra and selection rules, polarized and depolarized Raman lines, resonance Raman spectroscopy, use of symmetry to determine the number of active infrared and Raman lines, rotational fine structure in gas phase IR. Nonresonance overtones and difference bands. Application of Raman and Infrared selection rules to the determination of inorganic structures, bond strength frequency shift relations, changes in spectra of donor molecules on coordination, change in symmetry on coordination.

Mössbauer spectroscopy: Doppler shift and recoil energy, isomer shift and its interpretation, quadrupole interactions, effect of magnetic field on Mössbauer spectra, applications to metal complexes, metal carbonyls, Fe-S cluster and tin compounds, etc. Partial quadrupole splittings and geometry of the complexes.

Magnetism: Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems where $S = \frac{1}{2}$, van Vleck's equation, its derivation and its applications. Spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, T.I.P., intramolecular effects, antiferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria.

Mass spectrometry: Experimental arrangements and presentation of spectra, molecular ions, appearance and ionization potential, fragmentation, ion reactions and their interpretation, effect of isotopes on the appearance of a mass spectrum, molecular weight determination, thermodynamic data. Application of mass spectrometry to inorganic compounds.

Course-B: Electronic Spectroscopy, NMR, EPR and NQR Spectroscopy,

Electronic spectroscopy: Vibrational and electronic energy levels in a diatomic molecule, potential energy level diagram. Symmetry requirements for n to π^* transitions, oscillator strengths, transition moment integrals (electric dipole and magnetic dipole moment operator), selection rules, spin orbit and vibronic coupling contributions, mixing of d and p orbitals in certain symmetries. Polarized

absorption spectra. Survey of the electronic spectra of tetragonal complexes. Calculation of Dq and β for Ni(II) O_h complexes, nephelauxetic effect, effect of σ and π bonding on the energy of t_{2g} orbitals and Dq , spectrochemical series, effect of distortion on the d orbital energy level (T_d , D_{2d} , D_{4h}), *cis* and *trans* isomers and bonding parameters from spectra of tetragonal complexes, bonding parameters, calculation of Dq , Ds and Dt for tetragonal complexes, intervalence electronic transition, structural evidence from electronic spectra.

Nuclear magnetic resonance spectroscopy: Nuclear spin quantum number, I , and its calculation using

the nuclear shell model, spin parity rules. Types of nuclei based on value of I , nuclear spin angular momentum quantum number, and its relation to classical magnetic moment.

Behaviour of a bar magnet in a magnetic field. The NMR transition and NMR experiment, measuring chemical shifts, signal intensities and splitting. Application of chemical shifts, signal intensities and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei like ^1H , ^{11}B , ^{15}N , ^{19}F , ^{29}Si , ^{31}P , ^{183}W , ^{195}Pt , etc. Effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, the expectation value of $\langle S_z \rangle$, contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions. Contact shift and spin density, π delocalization, simplified M.O. diagram for Co(II) and Ni(II). Application to planar tetrahedral equilibrium, Contrast agents.

Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Shift operators and the second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Nuclear Quadrupolar Resonance (NQR) Spectroscopy: Quadrupolar moment, energy levels of a quadrupolar nucleus and effect of asymmetry parameters and energy levels. Effect of an external magnetic field, selected examples for elucidation of structural aspects of inorganic compounds using NQR spectroscopy.

Recommended Texts:

1. Kettle, S. F. A. *Physical Inorganic Chemistry: A Coordination Chemistry Approach*, Springer, Berlin, Heidelberg (1996).
2. Drago, Russell S. *Physical Methods for Chemists 2ed.* East West Press Pvt. Ltd. (2016).
3. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes.* Dover Publications; 2008 edition (2008).
4. Roberts, A. P. *Polyoxometalates: Properties, Structure and Synthesis*, Nova Science Publishers, Incorporated (2016).

Paper 4102- Inorganic Chemistry (Special-IV) (Elective Paper 2) (100 Marks/ 4 Credits)

Course A: Organotransition metal chemistry

General introduction, Structure and bonding, Survey of organometallic complexes according to ligands. π bonded organometallic compounds including carbonyls, nitrosyls, tertiary phosphines, hydrides, alkene, alkyne, cyclobutadiene, cyclopentadiene, arene compounds and their M.O. diagrams. Metal-carbon multiple bonds. Fluxional organometallic compounds including π -allyl complexes and their characterization. Metallocycles, unsaturated nitrogen ligands including dinitrogen complexes.

Futuristic aspects of organotransition metal chemistry.

Course B: Bio-inorganic chemistry

Fundamentals of inorganic biochemistry, geo-chemical effects on life systems, essential and non-essential elements in bio-systems.

Role of alkali/alkaline earth metals in bio-systems. Role of 3d block elements and nonmetals in bio-systems. Role of metal ions in oxygen carriers and synthetic oxygen carriers. Designing of chelating agents and metal chelates as medicines. Fixation of dinitrogen biologically and abiologically, biotransformation of nonmetallic inorganic compounds. Environmental bioinorganic chemistry. Metal ions as probes for locating active sites. Anti-

oxidants. Metal ions as antioxidants, metal ion enhancing catalytic activity of enzymes (Biocatalysts). Inhibitions as competitive and non-competitive, metals and metalloproteins.

Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). Template temperature, stability of DNA.

Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of dioxygen, bioinorganic chips and biosensors.

Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land.

Metals in the regulation of biochemical events. Transport and storage of metal ions *in vivo*.

Metal complexes as probes of structure and reactivity with metal substitution.

Fundamentals of Toxicity and Detoxification. Nuclear medicines.

Recommended Texts:

1. Green, M. L. H. *Organometallic Compounds* Chapman & Hall: U.K. (1968).
2. Coates, G. E., Green, M. L. H. & Powell, P. *Principles of Organometallic Chemistry* Chapman and Hall: U.K. (1988).
3. Lippard, S. J. & Berg, J. M. *Principles of Bioinorganic Chemistry* Univ. Science Books (1994).
4. Lippard, S. J. *Progress in Inorganic Chemistry* Vols. 18 and 38, Wiley-Interscience (1991).

Paper 4103- Inorganic Chemistry (Special-V) (Elective Paper 3) (100 Marks/ 4 Credits)

Course A: Analytical techniques (Instrumentation and Applications)

- (i) *Electroanalytical methods*:- Polarography (DC, AC and pulse), cyclic voltammetry, coulometry and anode stripping voltammetry.
- (ii) *Optical methods*:- UV/Visible, X-ray photoelectron spectroscopy (XPS), Auger Electron Spectroscopy (AES), ESCA, Atomic absorption and emission spectroscopy.
- (iii) *Infrared Spectroscopy*, Dispersive and Fourier Transformed Raman, Resonance Raman and Surface Enhanced Raman Spectroscopy- Dispersive and Fourier Transformed.
- (iv) *Hifanated Techniques*: GC-IR, TG-IR Spectroscopy, GC-Mass Spectroscopy and any other.
- (v) *Imaging Techniques*: Electron microscopy (SEM, TEM)

Course B: Diffraction, Separation and Thermal Methods

- (i) *Diffraction Methods*: Single crystal and Powder X-Ray Diffraction and their applications for Inorganic Compounds, Neutron Diffraction and Electron Diffraction.
- (ii) *Separation Methods*: Theory and applications of separation methods in analytical chemistry: solvent extraction, ion exchangers including liquid ion exchangers and chromatographic methods for identification and estimation of multicomponent systems (such as TLC, GC, HPLC, etc.).
- (iii) *Thermal Methods*: TG, DTA, DSC and thermometric titrations.

Recommended Texts:

1. West, A.R. Solid State Chemistry & its Applications, John Wiley & Sons (1987).
2. West, A.R. Basic Solid State Chemistry, 2nd Edition, John Wiley & Sons (2000).
3. Smart, L.E. & Moore, E.A. Solid State Chemistry - An Introduction, 3rd Edition, CRC Press (2005).
4. Rodgers, G.E. Descriptive Inorganic, Coordination & Solid-State Chemistry, 3rd Edition, Brooks/Cole, Cengage learning (2002).
5. Tilley, R.J.D. Understanding Solids: The science of materials. , 2nd Edition, John Wiley & Sons (2004).
6. Christian, G. D., Analytical Chemistry, 6th Ed., John Wiley & Sons, Inc. (2004).
7. Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A. *Principles of Instrumental Analysis* Saunders Golden Sunburst Series (1997).
8. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) *Instrumental Methods of Analysis* - 7th Ed., Wadsworth Publishing (1988) ISBN 0534081428
9. Cullity, B.D. & Stock, S.R. Powder X-Ray Diffraction, 3rd edition, Kindle Publisher 2001.
10. Stout, G.H. & Jensen, L. H. X- Ray structure Determination A Practical Guide Iied (John Wiley & Sons), 1989.

Paper 4104- Inorganic Chemistry (Special-VI/ Elective 4) (100 Marks/ 4 Credits)**Course A: Inorganic Materials**

Introduction to the solid state, metallic bond, Band theory (Zone model, Brillouin Zones, Limitations of the Zone model); Defects in solids, *p*-type and *n*-type; Inorganic semiconductors (use in transistors, IC, etc.); Electrical, optical, magnetic and thermal properties of inorganic materials. Superconductors, with special emphasis on the synthesis and structure of high temperature superconductors.

Solid State Lasers (Ruby, YAG and tunable lasers): Inorganic phosphor materials; Synthesis and advantages of optical fibres over conducting fibres. Diffusion in solids, catalysis and Zone refining of metals.

Preparation of nanomaterials and their characteristic differences over bulk materials. Principles of Electron Microscopy, Dynamic Light Scattering, Atomic Force Microscopy and characterization of nanomaterials.

Course B: Nuclear and Radiochemistry

Nuclear structure and nuclear stability, Nuclear models, Radioactivity and nuclear reactions (including nuclear fission and fusion reactions).

Hot atom chemistry, Nuclear fission and fusion reactors.

The interaction of nuclear radiations with matter. Radiation hazards and therapeutics.

Detectors and their principles.

The direction of radioactivity. The counting errors and their corrections.

Tracer techniques and their applications. Isotope dilution and radio-activation methods of analysis. Fission product analysis (e.g., the technique of isolating two or three different fission products of U or Th and determining the yields).

Recommended Texts:

1. West, A.R. Solid State Chemistry & its Applications, John Wiley & Sons (1987).
2. West, A.R. Basic Solid State Chemistry, 2nd Edition, John Wiley & Sons (2000).
3. Smart, L.E. & Moore, E.A. Solid State Chemistry - An Introduction, 3rd Edition, CRC Press (2005).

- Rodgers, G.E. Descriptive Inorganic, Coordination & Solid-State Chemistry, 3rd Edition, Brooks/Cole, Cengage learning (2002).
- Tilley, R.J.D. Understanding Solids: The science of materials, 2nd Edition, John Wiley & Sons (2004).
- Harvey, B. C. *Introduction to Nuclear Chemistry* Prentice-Hall (1969).
- Friedlander, G. Kennedy, J. W., Marcus, E. S. & Miller, J. M. *Nuclear & Radiochemistry*, John Wiley & Sons (1981).
- Timp, G., Ed. *Nanotechnology* Springer-Verlag: N. Y. (1999).

Paper 4105- Inorganic Chemistry (Special-VII/ Elective 4) (100 Marks/ 4 Credits)

Green Chemistry: An interdisciplinary approach towards sustainable development

Course A: Introduction to Green Chemistry

History of emergence of Green Chemistry through some industrial disasters, environmental movements for public awareness and some important environmental laws, Definition of Green Chemistry, Need for Green Chemistry, goals of Green Chemistry, Green Chemistry advances towards a sustainable future, Green Chemistry v/s Environmental Chemistry, Green Chemistry and its interdisciplinary nature, Twelve Principles of Green Chemistry and their illustrations with examples. Catalysis for Green Chemistry with examples. Catalytic oxidation using H₂O₂, Bio-catalysis, Photo-catalysis, Green reagents, Green solvents including solvent free synthesis of some organic compounds and inorganic complexes, alternative sources of energy, Green energy and sustainability.

Course B: Application of Green Chemistry in real world cases

Wealth from waste, Industrial case studies
 Green Nanotechnology, Greener approaches for nanoparticle synthesis
 Pharmaceutical industries: The largest waste producer problems and solutions through Green Chemistry benefits of greening industries, Need for Academia-Industry collaborations, Innovations stemming from Academia-Industry collaborations
 Emerging Green Technologies. Green solvents, Next generation catalyst design, Microwave assisted synthesis etc.

Suggested Texts:

- Anastas, P.T. & Warner, J.C. *Green Chemistry- Theory and Practical*, Oxford University Press (1998).
- Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
- Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
- Sharma, R.K. & Bandichhor, R. *Hazardous Reagent Substitution*, Royal Society of Chemistry, Green Chemistry Series (2018).
- Ryan, M.A. & Tinnes, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
- Sharma, R.K., Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiments: A Monograph* I.K. International Publishing House Pvt. Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7 (2013).
- Lancaster, M. *Green Chemistry: An Introductory Text* RSC publishing, 2nd Edition ISBN 978-1-84755-873-2 (2010).

PRACTICALS

Paper 4106- Practical Inorganic Chemistry – II (Elective practical 2) (200 Marks/ 8 Credits)*

Part – A: Analysis

Analysis of the following complex materials by various chemical methods:

- (i) Ores
- (ii) Alloys
- (iii) Inorganic substances
- (iv) Any other experiments done in the class during the current academic semester.

Part – B: Instrumental based Analysis:

Any three/four techniques not covered in the 3rd semester out of the following syllabus:

- (1) Instrumental methods of analysis utilizing flame photometer, atomic absorption spectrophotometer, pH-meter, potentiometer, turbidity meter, electrochemical methods, separation of mixtures of metal ions by ion exchange chromatography.
- (2) Synthesis and thermal analysis of group II metal oxalate hydrates.
- (3) Any other experiments done in the class during the current academic semester.

Organic Chemistry Special Papers

Paper 4201- Organic Chemistry (Elective course I) (100 Marks/ 4 Credits)

Course A: Advanced Organic Synthesis

Philosophy of organic synthesis: Disconnection approach, one group and two group disconnections, reversal of polarity, chemoselectivity, one group C-C disconnection, two group C-C disconnections, 1,3-difunctional and 1,5-difunctional compounds. Tandem reactions, Domino reactions and multi-component reactions.

Asymmetric synthesis: Development of methodologies for asymmetric synthesis, regioselectivity, stereoselectivity, diastereoselectivity and stereospecificity.

Total synthesis of the following compounds using disconnection approaches: Gingerol, (z)-jasmone, prostaglandins E₂, F₂ α , menthol, taxol and gandrionol.

Course B: Supramolecular Chemistry and Carbocyclic Rings

Principles of molecular associations and organizations: Non-covalent synthesis, Self assembly and self organization, Supramolecular reactivity and catalysis, Molecular devices, Ion channels, Novel liquid crystals, Gelators fibres and adhesives, Dendrimers, organic solids, organic conductors and organic superconductors, catenanes and rotaxanes.

Chemistry of small, medium and large ring compounds.

Chemistry of non-benzenoid aromatics: Tropones, tropolones, azulenes, metallocenes and annulenes. Bridged rings, caged molecules and adamantane.

Recommended Texts:

1. Warren, S. *Organic Synthesis: The Disconnection Approach* John Wiley & Sons (1984).
2. Lehn, J. M. *Supramolecular Chemistry: Concepts & Perspectives*, Print ISBN:9783527293124 Wiley-VCH (2006).
3. Vögtle, F. *Supramolecular Chemistry: An Introduction* John Wiley & Sons (1993).

Paper 4202- Organic Chemistry (Elective course 2) (100 Marks/ 4 Credits)

Course A: Terpenes and Steroids

Terpenes and steroids: Classification and biosynthesis of mono- sesqui-, di- and triterpenoids and steroids. Acetyl CoA, Mevalonic acid, acetoacetyl CoA, squalene to lanosterol, lanosterol to Cholesterol, Cholesterol to estradiol and progesterone, diosgenin and its utility in hormone synthesis.

General chemistry of the following compounds- Cholesterol, Artemisinin, Gibberellic acid, Azadirachtin.

Course B: Alkaloids and Polyphenols

Isolation and structure elucidation of alkaloids, Biosynthesis of alkaloids using thiokinase, mixed function oxygenases, methyl transferases, amino acid decarboxylases.

Total synthesis of morphine, reserpine and ergotamine.

Biosynthesis of flavonoids and related polyphenols. Synthesis of apigenin, luteolin, quercetin, Diadzein, myricetin, quercetin, prenylflavone, binaringenin and biflavonoids.

Recommended Texts:

1. Finar, I. L. & Finar, A. L. *Organic Chemistry* Vol. 2, Addison-Wesley (1998).
2. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).
3. Mann, J. *Secondary Metabolites*, Oxford University Press, Oxford, UK, (1980).

Paper 4203- Organic Chemistry (Elective course 3) (100 Marks/ 4 Credits)**Course A: Newer Synthetic Reactions and Reagents**

Enolates, Thermodynamic versus Kinetic enolates, enolate equivalents and enamines: Applications in carbon-carbon bond formation and related reactions. Applications in chiral synthesis.

Phosphorus, Sulphur and nitrogen ylides: Preparation, applications in organic synthesis and mechanism.

Umpolung reactions (sulphur compounds, nitro compounds, lithiated ethers and related compounds).

Principles and applications of phase transfer catalysis, crown ethers and polymer- supported reagents in organic synthesis.

Principles of Green Chemistry and its applications : Biotransformations: Classification of enzymes, advantages and disadvantages, Artificial enzymes, applications in organic synthesis; Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids.

Course B: Heterocyclic Chemistry

Introduction to heterocycles: Nomenclature, spectral characteristics, reactivity and aromaticity

Synthesis and reactions of three and four membered heterocycles, *e.g.*, aziridine, azirine, azetidene, oxiranes, thiarines, oxetenes and thietanes.

Five membered rings with two heteroatoms: pyrazole, imidazole, oxazole, thiazole, isothiazole and benzofused analogs.

Benzofused five membered heterocycles with one heteroatom, *e.g.* indole, benzofuran, benzothiophene.

Chemistry of bicyclic compounds containing one or more heteroatoms.

Benzofused six membered rings with one, two and three heteroatoms: benzopyrans, quinolines, isoquinolines, quinoxalines, acridines, phenoxazines, phenothiazines, benzotriazines, pteridines.

Seven and large membered heterocycles: azepines, oxepines, thiepinines. Chemistry of porphyrins and spiro heterocycles.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. Carruthers, W. *Modern Methods of Organic Synthesis* Cambridge University Press (1971).
3. Acheson, R. M. *Introduction to the Chemistry of Heterocyclic Compounds* John Wiley & Sons (1976).
4. Anastas, Paul and Warner, John C., *Green Chemistry- Theory and Practical*, (2005).
5. Alhuwalia, VK and Kidwai, M. *New trends in Green Chemistry*. Anamaya Publishers, New Delhi (2003).

Paper 4204- Organic Chemistry Special (Elective course 4) (100 Marks/ 4 Credits) Biomolecules

Course A: Proteins and Lipids

Peptides and proteins: Classification of naturally occurring peptides, depsipeptide and peptide alkaloids with examples, Sequence determination, chemical, enzymatic and mass spectral methods, Modern methods of peptide synthesis with protection and deprotection, Solid phase synthesis,

combinatorial synthesis of peptides, Chemistry of oxytocin, valinomycin, enkephalins, self assembly and aggregation of peptides,

Lipids : Classification and biological importance of fatty acids and lipids, stereochemical notation in lipids, chemical synthesis of phospholipids and glycolipids, properties of lipid aggregates, micelles, bilayers, lysosomes and biological membranes.

Course B: Nucleic Acids and Carbohydrates

Nucleic acids: Secondary structure of DNA and RNA, stabilizing forces, polymorphic nature of DNA, multistranded DNA structures, sequence determination by chemical and enzymatic methods, genome sequencing, chemical synthesis of DNA, solution phase and solid phase synthesis, phosphodiester-triester and phosphite methods, phosphoramidite approach; PNA, LNA, UNA, automated DNA synthesizers, purification of oligonucleotides, HPLC and gel electrophoresis.

Carbohydrates: Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, sugar methyl ethers and acid derivatives of sugars, polysaccharides of industrial and biological importance, dextran, chemistry of sialic acids, cell-cell recognition and blood group substances.

Recommended Texts:

1. Bodansky, M. *Peptide Chemistry: A Practical Textbook* Springer-Verlag (1988).
2. Dugas, H. & Penney, C. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action* Springer-Verlag (1989).
3. Stryer, L. *Biochemistry* 4th Ed., W. H. Freeman & Co. (1995).
4. Zubay, S. *Biochemistry* Addison-Wesley (1983).
5. Sinden, R. P. *DNA Structure and Function* Academic Press (1994).
6. Saenger, W. *Principles of Nucleic Acid Structure* Springer-Verlag (1984).
7. Gait, M. J., Ed. *Oligonucleotide Synthesis-A Practical Approach* IRL Press (1984).

Paper 4205- Organic Chemistry Special/ Elective course 4 (100 Marks/ 4 Credits)

Pharmaceutical Techniques Technologies Development

Course A: Drug Delivery Technologies

Importance of Targeted Drug Delivery, Efficacy, Safety and Toxicity Issues. Molecular basis of targeted drug delivery. Drug Release and Uptake Phenomenon. Drug Encapsulation Technologies. Different Carriers for Drug Encapsulation: Nanomaterials (metal-based, metal oxide based and polymeric) in drug encapsulation and drug delivery: their characterization, generation, efficacy, toxicity and release profile.

Factors affecting drug loading and drug release.

Techniques to measure degree of loading and release efficiency. Metabolism and excretion of drug delivery carriers.

General considerations; Methods of preparations, characterization and applications of liposomes, ionosomes, resealed erythrocytes, nanoparticulate systems, solid-liquid nanoparticles, dendrimers, organogels, multiple emulsions and nanoemulsions.

Overview and application of aquasomes, pharmacosomes, liquid crystalline systems, protein and peptide-based drug delivery systems.

Polymers in drug encapsulation and drug delivery: Classification, synthesis and applications of biodegradable and natural polymers in formulation of controlled drug delivery systems.

Course B: Pharmaceutical Technologies Development

Drug discovery, lead identification and lead optimization, Chemical, pharmaceutical and clinical technology development.

Investigational New Drug (IND) and its Applications : criteria, contents, categories, submission, regulation, noteworthy examples.

Clinical trials: Phase I, II and III clinical trials.

Pilot Plant Scale-Up Techniques: Primary function of the pharmaceutical pilot plant, factors to be considered during development, reporting responsibilities, personnel requirements, space requirements, review of the formula, raw materials, relevant processing equipments, production rates, process evaluation, master manufacturing procedures, GMP consideration, pilot plant design for tablet development.

Recommended Texts:

1. Mathiowitz, E., Ed. *Encyclopaedia of controlled delivery* (1999).
2. Joseph R. Robinson and Vincent H. L. Lee *Controlled Drug Delivery – Fundamentals and Applications*.
3. Saltzman, W. Mark *Drug Delivery: Engineering Principles and Drug Therapy* (Oxford Press)
4. Loyd V. Allen, Jr., Nicolas G. Popovich and Howard C. Arsel *Ansel's Pharmaceutical Dosage Forms and Drug Delivery Systems*.
5. *The Art, Science and Technology of Pharmaceutical Compounding* – Loyd V. Alen Jr.
6. *Theory and Practice of Industrial Pharmacy* – Lachmann
7. *Pharmaceutics* – Aulton

Paper 4206- Practical Organic Chemistry – II (Elective practical 2) (200 Marks/ 8 Credits)*

Part A

1. Separation and qualitative analysis of mixtures containing two components by chemical methods and physical methods (Separations using acids, bicarbonate bases, water, ether).
2. (i) Separation of active single component and mixture of components from pharmaceutical tablets; identification of components by m.p., functional groups and spectral data;
(ii) Quantitative estimation of the components in pharmaceutical tablets

2. Application of column chromatography, HPTLC, HPLC, GC etc.
3. Separation of DNA/Proteins by Gel- Electrophoresis
4. (i) Application of spectral data (IR, UV, NMR and mass) for structural elucidation,
(ii) Quantitative estimations of mixtures of compounds, geometrical isomers, keto-enol tautomers, etc.

Part B

1. Advanced organic synthesis:

Multistage synthesis including photochemical methods; representative examples:

 - a. Hydroquinone → Hydroquinone Diacetate → 2,5 -Dihydroxyacetophenone → 2, 5 -Dibenzoxyacetophenone
 - b. Benzaldehyde → Cinnamic acid → α,β -Dibromocinnamic acid → *cis* & *trans* α -Bromocinnamic acid
 - c. Chalcone → chalcone epoxide → α -Benzoyl phenyl acetaldehyde
 - d. Benzaldehyde → Bezoïn → Benzil → Benzilic acid
 - e. Resorcinol → 7-Hydroxy-4-methylcoumarin → 7-Acetoxy-4-methylcoumarin → 4-Methyl-7-hydroxy-8-acetylcoumarin
 - f. Applications of Grignard Reagent
 - g. Applications of Wittig reagent
 - h. Other suitable multi-step synthesis
2. Multi-component synthesis:
 - a. Mannich Reaction (reaction of primary amine, formaldehyde and carbonyl compound)
 - b. Organic synthesis in water (Preparation of Hydroxy methyl benzotriazole)
 - c. Synthesis of Benzimidazole (Condesation of diamines and aldehydes)
 - d. Synthesis of chromenes and xanthenes
 - e. Other recent examples of multi-component synthesis
3. Green chemistry:
 - a. Direct Oxidative esterification of Aldehyde (using Iodine and Alcohol).
 - b. Use of microwaves in organic synthesis
 - i. Synthesis of Chalcone
 - ii. Oxidation of toluene
 - iii. Esterification
 - iv. Lipase-catalyzed Esterification / transesterification reactions and other enzymatic reactions
 - v. Aldol condensation of Benzil
 - vi. And other suitable green synthesis
4. Supra-molecular chemistry

High dilution method for the synthesis of Host molecule, clatherates etc.

Physical Chemistry Special Papers

Paper 4301 –Physical Chemistry Special (Advanced Statistical Mechanics) (Elective course) (100 Marks/ 4 Credits)

Course A: Grand Canonical Ensemble:

Distribution functions in monatomic, one-component systems, Kirkwood-Salsburg integral equation, *Theory of Imperfect Gases and Condensation*

Partition functions and cluster integrals, Pressure of gas expressed as a power series in activity, Irreducible cluster integrals, Virial expansion for a gas, Calculation of Virial coefficients of an imperfect gas. Theory of condensation.

Lattice Statistics

Ising Model. Nearest neighbour lattice statistics- Thermodynamics and interconnections, Exact and formal methods.

Computational Techniques

Computer simulation: Motivation and applications, Intermolecular potentials

Molecular Dynamics and Monte Carlo Methods

Course B: Theory of Liquids

Canonical Ensemble: Definition of distribution and correlation functions, Thermodynamic functions of a fluid and the radial distribution function, Potential of mean force and the superposition approximation, Kirkwood integral equation, Born-Green-Yvon (BGY) integral equation, HNC equation, PY equation, Fluid of hard spheres according to the superposition approximation, Fluid with modified Lennard-Jones molecular interaction potential according to the superposition approximation.

Supercooled and Ionic Liquids

Theories of transport properties; non Arrhenius behaviour of transport properties, Cohen-Turnbull free volume model, configurational entropy model,

Experimental Methods for Structure Determination

Spectroscopic techniques for liquid structure studies, Neutron and X-ray scattering.

Recommended Texts:

1. Allen, M. P. & Tildesley, D. J. *Computer Simulations of Liquids* Oxford Science Publications: Oxford (1987).
2. Hill, T. L. *Statistical Mechanics: Principles and Selected Applications* Dover Publications Inc.: New York (1987).
3. Landau, L. D. & Lifshitz, E. M. *Statistical Physics* Vol. 5, Part 1, 3rd Ed., Pergamon Press (1980).
4. McQuarrie, D. A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
5. Bagchi B. *Statistical Mechanics for Chemistry and Material Science*, CRC Press (2018).

Paper 4302 –Physical Chemistry Special (Advanced Electrochemistry) (Elective course) (100 Marks/ 4 Credits)

Course A: Fundamentals

Electrode kinetics: Overpotentials, Exchange current density and transfer coefficient, Derivation of Butler-Volmer equation and its physical implications, Tafel plot, Multistep electrode reactions; Marcus microscopic model of electron transfer.

Relaxation Methods-Theory and Techniques: Mass transfer by diffusion and electrode surface constraints. Laplace transfer and its application to solve diffusion equation

Constant Potential Chronoamperometry: Reversible and quasi-reversible charge transfer, Cottrell equation, Influence of uncompensated solution resistance

Pulse Voltammetries: Reversible charge transfer

Constant Current Chronopotentiometry: Reversible and quasi-reversible charge transfer, Sand equation

Impedance Methods: Reversible and quasi-reversible charge transfer, Warburg equation, Influence of uncompensated solution resistance, Equivalent circuits models

Adsorption and Electric Double Layer:

Thermodynamics of the double layer, Electrocapillary phenomena;

Structure of electrified interfaces - Gouy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models;

Course B: Applications of Electrochemistry

Application of cyclic voltammetry for characterization of various electrochemical processes, Electrochemical instrumentations, Scanning probe techniques.

Conversion and storage of electrochemical energy: Fuel cells, Supercapacitors and Li ion batteries.

Electrocatalysis: Influence of various parameters on water splitting, HER and OER.

Corrosion: Introduction to corrosion, forms of corrosion, Corrosion monitoring and prevention methods

Semiconductor interfaces: Structure of double layer at the semiconductor-solution interface, Effect of light at semiconductor-solution interface. Dye sensitized solar cells

Electrocrystallization: Electrogrowth of metals on electrode- Nucleation, Growth, Surface Diffusion, Underpotential deposition, Variety of shapes formed in electrodeposition.

Bioelectrochemistry: Nerve impulses, Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, Core conductor model

Adsorption – Ionic and organic molecules, Adsorption isotherms - Langmuir, Frumkin, Temkin; Experimental evaluation of surface excesses and electrical parameters.

Recommended Texts:

1. Bard, A. J. Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., John Wiley & Sons: New York, 2002.
2. Oldham, K. B., Myland, J. C. and Bond, A. M. *Electrochemical Science and Technology: Fundamentals and Applications*, John Wiley & Sons, Ltd. (2012).
3. Bockris, J. O' M. & Reddy, A. K. N. *Modern Electrochemistry 1: Ionics* 2nd Ed., Springer (1998).
4. Bockris, J. O' M. & Reddy, A. K. N. *Modern Electrochemistry 2B: Electrodicts in Chemistry, Engineering, Biology and Environmental Science* 2nd Ed., Springer (2001).
5. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. *Modern Electrochemistry 2A: Fundamentals of Electrodicts* 2nd Ed., Springer (2001).
6. Brett, C. M. A. & Brett, A. M. O. *Electrochemistry*, Oxford University Press (1993).

7. Koryta, J., Dvorak, J. & Kavan, L. *Principles of Electrochemistry* John Wiley & Sons: NY (1993).
8. Bagotsky, V.S., *Fundamentals of electrochemistry* 2nd Ed. Wiley – Interscience, (2006)
9. Hamann, Carl H., Hamneff, Andrew & Vielstich, Wolf., *Electrochemistry*, 2nd Ed. (2007)

Paper 4303 –Physical Chemistry Special (Advanced Photochemistry and Radiation Chemistry)
(Elective course) (100 Marks/ 4 Credits)

Course A: Photochemistry

Molecular photochemistry: Transitions between states (Chemical, classical and quantum dynamics, vibronic states). Potential energy surfaces; transitions between potential energy surfaces, The Franck-Condon Principle and radiative transitions. A classical model of radiative transitions. The absorption and emission of light - state mixing, spin-orbit coupling and spin forbidden radiative transitions, absorption complexes, delayed fluorescence and phosphorescence.

Photophysical radiationless transitions: Wave mechanical interpretation of radiationless transitions between state factors that influence the rate of vibrational relaxation. Energy transfer: Theory of radiationless energy transfer, energy transfer by electron exchange: An overlap or collision mechanism. The role of energetics in energy transfer mechanism. Diffusion controlled quenching. The Perrin formulation. Triplet-triplet, triplet-singlet, singlet-triplet energy transfer. Multiphoton energy transfer processes, reversible energy transfer.

Course B: Radiation Chemistry, Dosimetry and Photolysis

An overview: G-value. The mechanism of interaction of high energy radiation with matter, Photoelectric effect, Compton effect, Pair production, total absorption co-efficient, excitation and ionization, Stopping power and linear energy transfer.

Radiation dosimetry: Radiation dose and its measurement, standard free air chamber method, chemical dosimeter (Frick's Dosimeter). Short lived intermediates (ions, excited molecules, free radicals: Various mechanisms of their formation and energy transfer processes).

Flash photolysis: Principle and its applications. Radiolysis of water and aqueous solutions. Radiolysis of molecules of biological interest (carbohydrates, amino acids, peptides, and nucleic acids).

Recommended Texts:

1. Turro, N. J. *Modern Molecular Photochemistry* Univ. Science Books (1991).
2. Gilbert, A. & Baggot, J. *Essentials of Molecular Photochemistry* Blackwell Scientific (1990)
3. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
4. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).

Paper 4304 –Physical Chemistry Special (Computational Methods in Chemistry)

(Elective course) (100 Marks/ 4 Credits)

Course A:

Programming: BASIC and FORTRAN/C languages. Introduction to LINUX/UNIX and shell scripts. Some illustrative numerical methods in chemistry: Least squares fit, root finding, numerical

differentiation, integration and solution of ODE, matrix inversion and diagonalization, interpolation. Pattern recognition techniques and molecular graphics.

Basics of electronic structure calculations, Molecular Mechanics, Monte Carlo and Molecular Dynamics simulations.

Course B:

Computer experiments: Use of some packages to study molecular electronic structures and molecular modelling (GAMESS, MOPAC, molecular dynamics packages, etc.) Use of electronic spreadsheets in chemistry. Basic ideas on structure-activity relationships, drug and catalysis design, etc. Development of some simulation programs and use of the internet for chemical information retrieval. Chemoinformatics.

Recommended Texts:

1. Hinchliffe, A. *Modelling Molecular Structures* 2nd Ed., John Wiley & Sons (2003).
2. Höltje, H-D., Sippl, W., Rognan, D. & Folkers, G. *Molecular Modeling: Basic Principles and Applications* 2nd Ed. Wiley-VCH (2003).
3. Leach, A. R. *Molecular Modelling: Principles and Applications*. 2nd Ed. Pearson Education: England (2001).
4. Press, W. H., Tenkolsky, S. A., Vetterling, W. T. & Flannery, B. P. *Numerical Recipes in Fortran/C* 2nd Ed., Cambridge University Press (1996).
5. Lewars, E. *Computational Chemistry* Kluwer Academic Publishers (2003)
6. Jensen, F. *Introduction to Computational Chemistry* Wiley (2007)
7. Cramer, C. J. *Essentials of Computational Chemistry* John Wiley & Sons, England (2002)

Paper 4305: Advanced Quantum Chemistry (Physical Chemistry Special)

(Elective course) (100 Marks/ 4 Credits)

Course A:

Perturbation theory- second order for non-degenerate states, first order for degenerate states. Double perturbation theory. Orbital and spin angular momentum operators of many-body systems, L-S and j-j couplings. Pauli matrices Term symbols and term energies. Hohenberg-Kohn theorem. Nature of electron density distribution and Density Functional Theories (DFT). Density functional interpretation of some concepts (electronegativity, electronegativity equalization, softness and hardness, etc). Electron correlation in DFT, Kohn-Sham equation and its applications. Quantum tunnel effect. Introduction to second quantization in chemistry, Fermi and Bose gases.

Course B:

Many-electron systems. Antisymmetrization, determinantal wavefunctions. Matrix elements for one and two electron operators. Secular equation for many-electron Slater determinantal functions, Hartree-Fock Self-Consistent-Field methods. Roothaan equations. Koopmans and Brillouin theorems. Basis sets (Slater, Gaussian and integral transform), Basis Set Superposition Error (BSSE), Electron correlation and CI theories. A review of HMO, EHT and PPP methods. ZDO approximation and CNDO, INDO and other semi-empirical theories.

Recommended Texts:

1. Lowe, J. P. & Peterson, K. *Quantum Chemistry* Academic Press (2005).
2. Mortimer, R. G. *Mathematics for Physical Chemistry* 2nd Ed. Elsevier (2005).

3. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
4. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
5. Atkins, P. W. & Friedman, R. S. Molecular Quantum Mechanics 3rd Ed., Oxford University Press (1997).
6. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
7. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).
8. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
9. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004).
10. Martin, R. M. Electronic Structure (basic theory and practical methods), Cambridge Univ. Press (2004).
11. Springborg, M. Methods of Electronic Structure Calculations, Wiley (2000).

Paper 4306 –Physical Chemistry Special (Advanced Chemical Kinetics)

(Elective course) (100 Marks/ 4 Credits)

Course A:

Statistical theories of kinetics: Collision theory. Activated Complex theory. Potential energy surfaces- attractive and repulsive forces. Lindemann's theory of unimolecular reactions- energy transfer, fall-off region and its limitations. Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular (isomerization) reactions.

Complex reactions: Chain reactions and oscillatory reactions, Photochemical reactions, Homogeneous catalysis.

Course B:

Enzyme kinetics: Michaelis-Menten mechanism - single and double intermediates. King-Altman method for working out the kinetics of complex enzyme reactions.

Enzyme inhibition- reversibility and products inhibition. Computer simulation in chemical kinetics.

Reaction Dynamics: Molecular beams, principle of crossed-molecular beams. Molecular encounters and principal parameters, e.g. Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity). Dependence of collisional cross-section on translational energy.

Probing the transition state, Dynamics of barrierless chemical kinetics in solution, dynamics of unimolecular reactions.

Recommended Texts:

1. Pilling, M. J. & Seakins, P. W. *Reaction Kinetics* Oxford Press (1997).
2. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).

Paper 4307 –Physical Chemistry Special (Advanced Molecular Spectra)

(Elective course) (100 Marks/ 4 Credits)

Course A:

Vibrational spectroscopy: Group theory and symmetry classification of normal modes of vibration. Normal coordinate analysis in Cartesian and internal coordinates of small molecules: BF₃, NH₃. Square planar, trigonal bipyramid, framework and cage molecules. Jahn-Teller distortions.

Electronic spectroscopy: Electronic spectroscopy of transition metal complexes. Octahedral and tetrahedral complexes, Correlation diagrams for octahedral fields and fields of lower symmetry.

Electronic spectroscopy of organic molecules - benzene, effect of substitution- pyridine, pyrimidine, pyrazine, methyl substitution. Vibronic analysis.

Course B:

Electron Spin Resonance spectroscopy: Basic principles. Relaxation and Line Widths. Zero-field splitting and Kramer's degeneracy. *g*-factor for paramagnetic ions. *g*-factor for organic radicals. Factors affecting the *g*-factor.

Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and McConnell relationship. Fine splitting in triplet spectra.

Applications of ESR spectroscopy - Structure determination, Interpretation of ESR spectra of simple organic radicals like benzene radical anion, naphthalene radical anion, toluene and *o*-, *m*- and *p*-xylene radical ions from HMO theory. Study of unstable paramagnetic species, Kinetic studies of electron transfer reactions, Spin-labelling studies of biomolecules.

Recommended Texts:

1. Harris, D. C. & Bertolucci, M. D. *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy* Dover Publications: New York (1990).
2. Bishop, D. M. *Group Theory and Chemistry*, Clarendon Press: Oxford, U.K. (1973).
3. Satyanarayana, D. N. *Handbook of Molecular Spectroscopy: From radio waves to gamma rays*, I.K. International Publishing House, New Delhi (2015).
4. Kakkar, R. *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).

Paper 4308 –Physical Chemistry Special (Crystal Structure)

(Elective course) (100 Marks/ 4 Credits)

Course A: Crystal Structures and Basic Symmetry

Overview: Description of a crystal structure in terms of atom positions, unit cells, and crystal symmetry; Relation of the crystal symmetry to the symmetry observed in a diffraction experiment for primitive, orthorhombic, tetragonal, trigonal, hexagonal, and cubic crystal systems. Concept of Reciprocal space.

Scattering and Diffraction Theory

X-ray Diffraction: Interaction of radiation with condensed matter and how this can be used in generalized crystallography. Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, Structure factor and its relation to intensity and electron density, Fourier synthesis. Phase problem, Patterson synthesis. Heavy atom method. Direct method. Refinement, R factor. Fourier refinement.

Least squares refinement. Determination of absolute configurations (Bijvoet method). Chemical interpretation of results. Estimation of errors. Effects of thermal motion, limitations. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

Crystal defects and non-stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies- Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

Course B:

Protein Crystallography

Basics of modern protein crystallography using Web-based material; different levels of structure exhibited by proteins; instrumentation, steps, and methods used in protein crystallography with appropriate case studies; concept of non-crystallographic symmetry to protein crystallography, Ramachandran diagram.

Electronic properties and Band Theory: Metals, insulators and semiconductors, electronic structure of solids- band theory, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductors, *p-n* junctions, super conductors.

Magnetic properties- Classification of materials: Quantum theory of paramagnetics - cooperative phenomena - magnetic domains, Hysteresis.

Organic solids: Electrically conducting solids, organic charge transfer complexes, organic metals, new superconductors.

Electron Microscopy: Fundamentals of electron microscopy as a useful subsidiary technique for crystallographers; Examples of its application in materials science and macromolecular structural biology.

Electron diffraction: Scattering intensity *versus* scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cells.

Recommended Texts:

1. Moore, E. & Smart, L. *Solid State Chemistry: An Introduction* 2nd Ed. Chapman & Hall (1996)
2. Rhodes, G. *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models* 3rd Ed. Elsevier (2006)
3. Massa, W. *Crystal Structure Determination* 2nd Ed. Springer (2004).
4. Warren, B. E., *X-Ray Diffraction* 1st Ed. Dover Publications (1990).
5. Sands, D. E. *Introduction to Crystallography* Reprint Dover Publications (1994).

Paper 4309 –Physical Chemistry Special (Macromolecules)

(Elective course) (100 Marks/ 4 Credits)

Course A: Fundamental of Single Chain, Solutions, Gels and Melts

Properties of an isolated polymer molecule: Ideal chain, Freely joined Gaussian chain, Distribution of segments in polymer chain, non ideal chain, excluded volume, Dimension of real chains and scaling laws, Self-avoiding walk

Concentrated solution and melts: Thermodynamic properties of polymer solutions, concentration fluctuation in polymer solutions, polymer blends, block copolymer

Polymer gels: Elasticity of rubber, Stress optical law, interaction between partial chains, swelling of gels

Molecular motion of polymers in dilute solution: General theory of Brownian motion, Rouse and Zimm Bead spring models, hydrodynamics interactions, dynamic light scattering

Molecular motion in entangled polymer systems: Qualitative aspects

Course B: Microstructure, Kinetics and Electrically Conducting Polymer

Polymer microstructure: Microstructure based on chemical structure and geometrical structure. Meaning of glass transition temperature (T_g), factors influencing the glass transition temperature, importance of glass transition temperature T_g and molecular weight, T_g and melting point

Structure of macromolecules: Polymer crystals: crystallization in polymers, factors determining crystal structure. Morphology of solution grown single crystal and bulk grown crystal. Semi-crystalline polymers: spherulites, degree of crystallinity, crystallization and melting. Kinetics of crystallization. Molecular mechanism of crystallization, factors affecting melting.

Kinetics of polymerization: Kinetics and statistics of step growth polymerization, size distribution in linear polymers, nonlinear polymerization and prediction of gel point. Kinetics of free radical chain polymerization, cationic polymerization, anionic polymerization and polycondensation.

Electrically conducting polymers: Discovery of electrically conducting polymers, Factors affecting the conductivity of conducting polymers. Electrochemical polymerization. Nature of charge carriers in conducting polymers: solitons, polarons and bipolarons. Mechanism of conduction in polymers.

Stimuli-sensitive (smart) polymers: pH- and temperature-sensitive smart polymers and their applications in biotechnology and medicine.

Recommended Texts:

1. Teraoka, I., Polymer Solutions, Wiley-Interscience, A John Wiley & Sons Inc. (2002).
2. Doi, M., The Introduction of Polymer Physics, Clarendon Press Oxford (1995).
3. DeGennes, P. G. *Scaling Concepts in Polymer Physics* Cornell University Press (1979).
4. Young, R. J. & Lovell, P. A. *Introduction to Polymers* 2nd Ed. Chapman & Hall (1991).

Paper 4310 –Physical Chemistry Special (Biophysical Chemistry)

(Elective course) (100 Marks/ 4 Credits)

Course A: Fundamentals of biological macromolecules

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; polypeptide chain geometries and internal rotational angles; Ramachandran plots; Structures of nucleic acids. Protein structure and function. Stabilizing interactions in biomolecules; Properties of nucleosides and nucleotides; composition of nucleic acids.

Methods for the separation of biomolecules: General principles, including Chromatography; Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

Course B: Conformational analysis and structural determinations

Complexities in modelling macromolecular structure; Molecular mechanics; simulating macromolecular structure; energy minimization; Molecular Dynamics.

Physical methods: Ultracentrifugation and other hydrodynamic techniques; Light scattering, fundamental concepts, scattering from a number of small particles: Rayleigh scattering, scattering from particles that are not small compared to the wavelength of radiation; Dynamic light scattering; Low angle X-Ray scattering; Neutron scattering; Raman scattering

Optical methods and applications: Optical techniques in biological systems: Absorption spectroscopy, Fluorescence spectroscopy, Linear and Circular Dichroism, Single and multidimensional NMR spectroscopy. Single molecule spectroscopy of biomolecules.

Recommended Texts:

1. Cantor, C. R. & Schimmel *Biophysical Chemistry* Vols. 1-3, W. H. Freeman (1980).
2. Lehninger, A. L., Nelson, D. L. & Cox, M. M. *Lehninger Principles of Biochemistry* 4th Ed., W. H. Freeman (2004).

**Paper 4311 –Physical Chemistry Special (Physical Chemistry of Materials)
(Elective course) (100 Marks/ 4 Credits)**

Course A: Soft Materials

Thin Films and Langmuir-Blodgett films

Preparation techniques, evaporation/sputtering, chemical processes, MOCVD, sol-gel, etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Liquid crystals: Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases, smectic-nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular rearrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Colloids: Types of colloids, forces between colloidal particles, characterization of colloids, charge stabilization, steric stabilization, effect of polymer on colloid stability, kinetic properties, sols, gels, clays, foams, emulsions, food colloids, concentrated colloidal dispersions.

Polymer: Polymer melts- The tube model, viscoelastic behaviour, experimental observations of single chain dynamics- Rouse and Zimm models, polymer blends, copolymers, incompatibility and segregation.

Course B: Glasses, Ceramics, High Tc Materials and Devices

Glasses, ceramics, composites and nanomaterials. Glassy state, glass formers and glass modifiers, Applications. Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications.

Microscopic composites, dispersion strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

Ionic conductors: Types of ionic conductors, mechanism of ionic conduction, interstitial types (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

High T_c materials: Defect perovskites, high T_c superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-paying and multigap structure in high T_c materials, applications of high T_c materials.

Materials for solid-state devices: Rectifiers, transistors, capacitors IV-V compounds, low-dimensional quantum structures; optical properties.

Organic solids, fullerenes, molecular devices: Conducting organics, organic superconductors, magnetism in organic materials.

Fullerenes - doped fullerenes as superconductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches- sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order- molecular hyperpolarizability and second order electric susceptibility- materials for second and third harmonic generation.

Recommended Texts:

1. Ashcroft, N. W. & Mermin, N. D. *Solid State Physics* Holt-Saunders (1976)
2. Callister, W. D., Jr. *Materials Science & Engineering: An Introduction* John Wiley & Sons: New York (2000).
3. Keer, H. V. *Principles of the Solid State* Wiley Eastern Ltd.: New Delhi (1993).
4. Gray, G. W., Ed. *Thermotropic Liquid Crystals* John Wiley & Sons: New York (1987).
5. Serpone, N. & Pelizzetti, E. *Photocatalysis: Fundamentals and Applications* John Wiley & Sons (1989).
6. Cowie, J. M. G. *Polymers: Chemistry and Physics of Modern Materials* 2nd Ed. CRC Press (1991)
7. Hamley, I. W. *Introduction to Soft Matter: Polymers, Colloids, Amphiphiles and Liquid Crystals* John Wiley & Sons (2000).

(Note: Papers belonging to physical chemistry teaching in semester-IV may combine any two parts, viz. course A or course B, of same or different elective papers (4301 to 4311). These combined courses will form 4 elective papers. Available elective papers will be displayed on the web site of Department of Chemistry before the beginning of the semester.)

Paper 4312- Practical Physical Chemistry- II (Elective practical 2) (200 Marks/ 8 Credits)*

Set A

COMPUTER PROGRAMMING

BASIC programming

1. Numerical methods and their applications in chemistry
2. Some typical exercises based on the above
 - i. Decimal-binary conversion
 - ii. Numerical differentiation, quadrature and finding roots

- iii. pH of a weak acid
- iv. Roots of cubic equations (e.g. van der Waals' equation)- iterative, Newton-Raphson, Binary bisection, Regula-Falsi methods.
- v. Titration curves and end-point location
- vi. Numerical integration (Trapezoidal, Simpson's rule)
- vii. H and S from C_p data
- viii. Chemical kinetics simulations
- ix. Least-squares fit including graphics
- x. Numerical solution of differential equations (e.g. in kinetics)
- xi. Intrapolation & interpolation of data
- xii. Gauss-Siedel method and its use in solving simultaneous equations (e.g. Lambert-Beer's law)

Set B

SPECTROPHOTOMETRY

1. Record the UV spectra of a weak acid (p -nitrophenol in 1:4 ethanol:water mixture) at different pH and determine the dissociation constant in the ground state.
2. (a) Record the UV spectra of a weak acid (α -naphthol) at different pH and determine the dissociation constant in the ground state.
(b) Record the fluorescence spectra of a weak acid (α -naphthol) at different pH and determine the dissociation constant in the excited state.
Comment on the difference in the two values using MO theory.
3. (a) Record the UV spectra of methyl orange at different pH and determine its dissociation constant.
(b) Study the effect of surfactant on the pK_a value of methyl orange.
4. Find the stoichiometry of the charge transfer (CT) complex formed between thiocyanate ions and iron(III) by Job's method of continuous variation. Determine the concentration equilibrium constant and extinction coefficient for the charge transfer complex by applying the Benesi-Hildebrand equation.
5. Repeat Expt. 4 for salicylate ions in place of thiocyanate ions.
6. Record the UV spectra of benzene, pyridine and pyrimidine in methanol. Compare and discuss the various transitions involved in terms of MO theory.

SET C

CYCLIC VOLTAMMETRY, IMPEDANCE, CHRONOPOTENTIOMETRY, EIS DATA ANAYSIS AND SIMULATIONS

CYCLIC VOLTAMMETRY

1. Reset the CV of aqueous solution of sulphuric acid (0.5 M) at Pt electrode as working electrode and counter electrode.
(a) Interpret and explain various peaks and regions of the CV and their significance.
(b) Determine the area and roughness factor of the electrode by H-adsorption and H-desorption.
(c) Determine the area and roughness factor of the electrode by Pt oxide region.
2. Determine the extent of catalytic activity of the Pt electrode by H_2 evolution reaction (HER) and O_2 evolution reaction (OER).

IMPEDANCE

3. Verify Warburg equation using electrochemical impedance spectroscopy. Perform experiment with various bias potentials around CV peak potential.
4. Determine the exchange current density, α (symmetry factor) and double layer capacity of a redox reaction using platinum electrode (aqueous solution of 10 mM $(\text{Fe}(\text{NH}_4)_2(\text{SO}_4)_2 + \text{Fe}(\text{NH}_4)_2(\text{SO}_4)_2)$ in 1 M HClO_4).

CHRONPOTENTIOMETRY

5. (a) Verify the Sand equation using galvanostatic chronopotentiometry.
- (b) The surface area of an electrode is determined via a chronopotentiometric measurement.
- (c) Determine the diffusion coefficient of the ion $[\text{Fe}(\text{CN})_6]^{3-}$

EIS DATA ANALYSIS AND SIMULATIONS

6. Determine the best fit model from electrochemical EIS data and extract electrochemical system parameters from the given impedance data using equivalent circuit models, viz. Resistor capacitor, Randles, Warburg, CPE, CPE with diffusion, etc.

Set D

COLOURIMETRY, DIGITAL POLARIMETRY

COLOURIMETRY

1. Study the kinetics of oxidation of isopropyl alcohol/ ethanol by potassium dichromate. Determine the order, rate constant, energy of activation and possible mechanism for the reaction.
2. Find the stoichiometry of the complex formed between a metal ion (Fe^{3+}) and a ligand (salicylate) by Job's continuous variation method and determine the stability constant of the complex formed.
3. Find the stoichiometry of the complex formed between a metal ion (Fe^{3+}) and a ligand (thiocyanate) by Job's continuous variation method and determine the stability constant of the complex formed.
4. Study the kinetics of hydrolysis of 4-nitrophenyl ethanoate in the presence of base.
5. Determine the dissociation constant of an indicator (methyl red) *colourimetrically*.

DIGITAL POLARIMETRY

6. Determine the velocity constant for the mutarotation of D(+) glucose and determine the order of the reaction and the equilibrium concentrations of the two forms.
7. (a) Determine the specific rotation constant for sucrose.
- (b) Study the acid catalyzed inversion of cane sugar, and find out
 - (i) the order with respect to sucrose;
 - (ii) the rate constant;
 - (iii) Compare kinetically the strengths of two acids (HCl and H_2SO_4)

SET E

PHOTOCHEMISTRY & NANOSCIENCE

1. Determine the intensity of light from a UV source using the reaction between Fe^{3+} and oxalate ions by photosensitization-Ferrioxalate actinometer.
- 2.(a) Study the photochemical decomposition reaction of cyclohexanone pH-metrically.
- (b) Study the above reaction conductometrically.
3. Prepare the transition metal complex cyano acid of potassium ferrocyanide (or ferricyanide) by the

ion-exchange method.

- (a) Determine the nature of this acid by the conductometric method.
- (b) Study the titration curves of the photolyzed acid (UV radiation), and suggest a possible mechanism for its decomposition.

NANOSCIENCE

4. (i) Determine the rate constant of the redox reaction between hexacyanoferrate and thiosulphate ions in the presence and absence of gold nanoparticles.
 - (ii) Determine the temperature coefficient, activation energy and other thermodynamic parameters of the reaction.
 5. Prepare gold nanostructures by reducing auric chloride with tea extract in presence of CTAB as capping agent, and characterize spectrophotometrically.
 6. Prepare CdS nanoparticles and record their UV/Vis spectra.
 7. Prepare CdSe quantum dots and record their absorption and emission spectra.
- (*Note: Depending on availability of time, some experiments may be added/deleted during the semester. II & IV semester experiments may be interchanged depending on availability of instruments.*)

Recommended Practical Chemistry Manuals and Books:

1. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis* - 7th ed. (revised by G. Svehla) Longmans (1996) ISBN 058-221866-7
2. Vogel, A. I. *Vogel's Textbook of Quantitative Chemical Analysis* - 5th Ed. Longman (1989).
3. Addison Ault *Techniques and Experiments for Organic Chemistry* 6th Ed. University Science Books (1998).
4. Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry* 4th Ed. Orient Longmans (1990).
5. Vogel, A. I. *Vogel's Textbook of Practical Organic Chemistry* 5th Ed. (revised by A.R. Tatchell *et al.*) Wiley (1989) ISBN 0582-46236-3
9. Daniels, F., Williams, J. W., Bender, P., Alberty, R. A., Cornwell, C. D. & Harriman, J. E. *Experimental Physical Chemistry*, McGraw-Hill (1962).
10. Das & R. C. & Behera, B., *Experimental Physical Chemistry*, Tata McGraw-Hill Publishing Co. Pvt. Ltd. (1993).
11. Shoemaker, D. P., Garland, C. W. & Nibler, J. W. *Experiments in Physical Chemistry*, McGraw-Hill: New York (1996).
12. Day, R. A., Jr. & Underwood, A. L. *Quantitative Analysis* 3rd Ed. Prentice-Hall India Pvt. Ltd.: New Delhi (1977).
13. Burns, D. T. & Rattenbury, E. M. *Introductory Practical Physical Chemistry* Pergamon Press (1966)
14. Harris, D. C. *Quantitative Chemical Analysis* 6th Ed. W. H. Freeman & Co. (2002).
15. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) *Instrumental Methods of Analysis* - 7th Ed., Wadsworth Publishing (February 1988) ISBN 0534081428
16. Noggle, J., *Physical Chemistry Using Mathcad* Newark, DE, 1997.
17. Rogers, D. *Computational Chemistry Using the PC*, 3rd Edition Wiley-Interscience (2003).
18. Quinn, C.M. *Computational Quantum Chemistry*, Series, Academic Press (2002).
19. Holze, R. *Experimental Electrochemistry*, John Wiley & Sons (2009)

Research Training during M.Sc. Chemistry Course

Science in the 21st century is rich with opportunity and challenges. Our pillars for success in this complex world are all tied to interactions—between people and between disciplines. By building both strong interpersonal connections between our students and faculty, and effective bridges between disciplines, entering Master degree students in the Department of Chemistry can thrive at the frontiers of research if research is pursued at interface of chemistry and Biology. *Hence we must start **Chemical Biology** as one of the specialization at master degree level, which would facilitate collaboration and cross-disciplinary research.*

Research should be primary focus of our Master's degree programs, with students choosing faculty as Advisors and beginning active research during their first year. Our faculty must share with M.Sc students a rich training in the unique tools of chemical inquiry and a commitment to scientific investigation at the molecular level. For their initial research, we must encourage students to explore problems of intrinsic interest and importance at the frontiers of chemical science. We must offer many opportunities for interdisciplinary studies. Interaction with other departments and groups is common, both within University of Delhi and at other research Centers in the University and neighbouring area. Thesis research will become a significant focus following an initial period of coursework, teaching, and sampling of research opportunities through our laboratory rotation system

Therefore, Department of Chemistry has decided to have **Master's degree (M.Sc) in Chemistry** with specialization in: **Inorganic, Chemistry, Physical for this year.**

However, from next year the department propose to have additional specializations at M.Sc level, viz: Chemical Biology, Material Science, Computational Chemistry and Analytical Chemistry.

Department of Chemistry has also decided to attach each and every M.Sc (F) student with a faculty member to complete a research project work of 100 marks (4 credits), based on an original piece of research. It may kindly be included in the preamble of the Syllabi of our M.Sc Chemistry.

In addition, it is proposed that the Faculty of Science should provide some compulsory Auditing Courses for M.Sc students across the faculty, like:

1. Ethics Education in Science
2. Lab Safety
3. IPR (Intellectual Property Right)
4. Research Methodology
5. Law in Science or Science and Law
6. Molecular Modelling & Computational Biology
7. Forensic Chemistry