ST. JOSEPH’S COLLEGE
(AUTONOMOUS), IRINJALAKUDA

M.Sc. DEGREE PROGRAMME
IN
CHEMISTRY

SCHEME AND SYLLABI

2018 ADMISSION ONWARDS

M.Sc. CHEMISTRY (CSS PATTERN)

Regulations and Syllabus with effect from 2018 admission

The Board of Studies in Chemistry (PG) at its meeting held on 24-11-2017 considered the revision of M.Sc. Chemistry syllabus under Credit Semester System (CSS) and resolved to implement the revised syllabus from 2018 admission onwards. The revised programme pattern; syllabus, distribution of credits and scheme of evaluation, etc. approved by the Board of studies in Chemistry (PG) at its meeting held on 24-11-2017 are given below:

Pattern of the Programme

a) The name of the programme shall be M.Sc. Chemistry under CSS pattern.

b) The programme shall be offered in four semesters within a period of two academic years.

c) Eligibility for admission will be as per the rules laid down by the University from time to time.

d) Details of the programme offered for the programme are given in Table 1. The programme shall be conducted in accordance with the programme pattern, scheme of examination and syllabus prescribed. Of the 25 hours per week, 12 hours shall be allotted for theory, 12 hours for practical and 1 hour for seminar.

Theory Courses

In the first three semesters there will be four theory courses and in the fourth semester three theory courses. All the theory courses in the first and second semesters are core courses. In the third semester there will be three core theory courses and one elective theory course. Colleges can choose any one of the elective courses given in the table 1. In the fourth semester there will be two core theory courses and one elective theory course. Colleges can select any one of the elective courses from those given in the table 1. However a student may be permitted to choose any other elective course in the third and fourth semesters, without having any lecture classes. Only one elective course chosen by the college both in the third and fourth semesters will be considered for calculating the workload of teachers. All the theory courses in the first, second and third semesters are of 3 credits while the theory courses in the fourth

semester are of 4 credits

Practical Courses

In each semester, there will be three core practical courses. However the practical examinations will be conducted only at the end of second and fourth semesters. At the end of second semester, three practical examinations with the codes CH1PO1 & CH2PO4, CH1PO2 & CH2PO5 and CH1PO3 & CH2PO6 will be conducted. Practical examinations for the codes CH3PO7 & CH4P10, CH3PO8 & CH4P11 and CH3PO9 & CH4P12 will be conducted at the end of fourth semester. Each practical examination will be of six hour duration and 4 credits. Three hours per week in the fourth semester are allotted for conducting individual project work by the students under guidance of a faculty and it can be treated as practical hours while working out the workload of teachers.

Project and Viva Voce

Each student has to perform an independent research project work during the programme under the guidance of a faculty member of the college/ scientists or faculties of recognised research institutions. Projects done in the quality control or quality analysis division of the industries will not be considered. At the same time, projects done in the R & D division of reputed industry can be considered. Each student has to submit three copies of the project dissertation for valuation at the end of fourth semester. After the valuation one copy may be returned to the student, one may be given to the project supervisor and the third one should be kept in the department/college library. Evaluation of the project work (4 credits) will be done on a separate day at the end of fourth semester, after the theory examinations. Viva voce on the project will also be done on the same day.

Viva voce examinations, based on the theory and practical courses, will be conducted at the end of second and fourth semesters (2credits each), on a separate day.

PROGRAMME OUTCOME

- Generate and interpret scientific data using quantitative, qualitative and analytical methodologies and techniques
- Apply contemporary research methods, skills and techniques to conduct independent inquiry in a chosen scientific discipline.

PROGRAMME SPECIFIC OUTCOME

- To familiarize the emerging areas of chemistry and their applications in various spheres of chemical sciences and to apprise the students of its relevance in future studies.

- To develop skills in the proper handling of instruments and chemicals.
- To be exposed to the different processes used in industries and their applications.
- To develop the ability for applying the principles of chemistry

Grading and Evaluation

(1) Accumulated minimum credit required for successful completion of the course shall be 80.

(2) A project work of 4 credits is compulsory and it should be done during the programme. However specific hours(3hours/week) are given in the IV semester, for project work. Project evaluation should be conducted by three external examiners, one each from inorganic chemistry, organic chemistry and physical chemistry area, at the end of IV semester, on a separate day.

Also comprehensive Viva Voce may be conducted by three external examiners, one each from inorganic chemistry, organic chemistry and physical chemistry area, at the end of II and IV Semesters on a separate day and carries 2 credits each.

(3) Evaluation and Grading should be done by direct grading system. All grading during the evaluation of courses and the semester is done on 5 point scale (A, B, C, D, E). Grading in 5 point scale is as given below.

Overall Grade in a course/Semester

GPA/SGPA	*Overall Letter Grade*
3.50 to 4.00	A
2.50 to 3.49	B
1.50 to 2.49	C
0.50 to 1.49	D
0.00 to 0.49	E

Pass in a course: C grade and above(GPA 1.50 and above). Pass in all courses in a semester is compulsory to calculate the SGPA.

GPA, SGPA and CGPA – between 0 to 4 and in two decimal points. An overall letter grade (Cumulative Grade) for the whole programme shall be awarded to the student based on the value of CGPA using a 7-point scale given below.

Overall Grade in a Programme

CGPA	*Overall Letter Grade*
3.80 to 4.00	A+
3.50 to 3.79	A
3.00 to 3.49	B+
2.50 to 2.99	B
2.00 to 2.49	C+
1.50 to 1.99	C
1.00 to 1.49	D

(4) Weightage of Internal and External valuation:

The evaluation scheme for each course shall contain two parts (a)) internal evaluation

(b) external evaluation. Its weightages are as follows:

Evaluation	*Weightage*
Internal	1 (or 25%)
External	3 (or 75%)

Both internal and external evaluation will be carried out using Direct Grading System, in 5 point scale

(5) Internal evaluation (must be transparent and fair):

Theory: 5 weightage

a) Internal Examinations- weightage = 2 (2 internal exams, both should be consbe considered)

b) Assignments and Exercises- weightage =1

c) Seminars and Viva Voce- weightage =1

d) Attendance - weightage =1

Practical: 5 weightage

a) Attendance - weightage =1

b) Lab. skill/quality of their results- weightage =1

c) Model practical test-weightage= 1 (Best one, out of two model exams is considered)

d) Record – weightage = 1

e) Viva Voce- weightage =1

Project: 5 weightage

a) Literature survey and data collection -weightage=2

b) Interpretation of data & Preparation of Project report - weightage =1

c) Research attitude - weightage = 1

d) Viva Voce- weightage =1

Project internal evaluation of each student should be done by the supervising faculty in the department.

Viva Voce: No internal evaluation for viva voce examinations (at the end of 2nd and 4th semesters).

Attendance: Above 90%: A, 85 – 89.99% : B, 80 – 84.99%: C, 75 -79.99%: D

Less than 75%: E

(6) External evaluation:

a) **Theory**: In all semesters the theory courses have 36 weightage each. Pattern of question Papers for theory courses is as follows

Division	*Type*	*No.of Questions*	*Weightage*	*Total Weightage*
Section A	Short Answer	12 (No Choice)	1	12
Section B	Short Essay	8 out of 12	2	16
Section C	Essay	2 out of 4	4	08
		Total weightage in a question paper		**36**

b) **Practicals**: At the end of II and IV semesters. There will be three practical examinations at the end of second semester as well as at the end of fourth semester. Each examination has 15 weightage and 4 credits

c) **Viva Voce**: At the end of II and IV semesters on a separate day(2credits each). Viva voce will be based on both the theory and practical courses during the year.

d) **Project Evaluation**: End of IV semester on a separate day. Evaluation is based on:

a Sigificance and relevance of the project-weightage=3
b Project report - weightage =6
c Presentation- weightage = 3
c) Viva Voce- weightage =3

Total weightage 15 and credit for project is 4.

(7) Directions for question paper setters:

Section A: Set each questions to be answered in 5 minutes duration.

Section B: 10 minutes answerable questions each. May be asked as a single question or parts.

Section C: 20 minutes answerable questions each. May be asked as a single question or parts.

While setting the question paper, all units in each theory courses must be given due consideration and should give equal distribution as possible.

(Furthur details regarding the grading and evaluation are as per the University PG regulations 2010)

Dr. Jessy Emmanuel
Chairman,
Board of Studies (Chemistry PG)
St.Joseph's College(Autonomous), Irinjalakuda

TABLE 1

Courses offered for M.Sc. Chemistry Programme under CSS Patten in Affiliated Colleges (2018 onwards)

Semester	Course Code	Course Title	Instruction/ Week	Credits
I	CH1CO1	Basic concepts in quantum chemistry and group Theory	3	3
	CH1CO2	Elementary inorganic chemistry	3	3
	CH1CO3	Structure and reactivity of organic compounds	3	3
	CHICO4	Thermodynamics, kinetics and catalysis	3	3
	CH1PO1	Inorganic chemistry practical I	4	-
	CH1PO2	Organic chemistry Practical I	4	-
	CH1PO3	Physical chemistry practical I	4	-
		Total credits:	**Core**	**12**
II	CH2CO5	Applications of quantum mechanics and group theory	3	3
	CH2CO6	Coordination chemistry	3	3
	CH2CO7	Organic reaction mechanisms	3	3
	CH2CO8	Electrochemistry, solid state chemistry and Statistical Thermodynamics	3	3
	CH2PO4	Inorganic chemistry practical II	4	4
	CH2PO5	Organic chemistry practical II	4	4
	CH2PO6	Physical chemistry practical II	4	4
	CH2VO1	Viva voce		2
		Total credits:	**Core** **Viva**	**24** **2**
III	CH3CO9	Molecular spectroscopy	3	3
	CH3C10	Organometallic &Bioinorganic chemistry	3	3
	CH3C11	Organic transformations and reagents	3	3
	CH3PO7	Inorganic chemistry practical III	4	
	CH3PO8	Organic chemistry practical III	4	
	CH3PO9	Physical chemistry practical III	4	
	CH3EO1	Synthetic organic chemistry(Elective)	3	3
		Total Credits:	**Core** **Elective**	**9** **3**

	CH4C12	Advanced Topics in Chemistry	4	4
	CH4C13	Instrumental Methods of Analysis	4	4
	CH4P10	Inorganic Chemistry Practical IV	3	4
	CH4P11	Organic Chemistry Practical IV	3	4
	CH4P12	Physical Chemistry Practical IV	3	4
	CH4EO5	Industrial Catalysis(Elective)	4	4
	CH4PrO1	Research Project	3	4
	CH4VO2	Viva Voce		2
IV		**Total Credits:**		
			Core	**20**
			Elective	**4**
			Project	**4**
			Viva	**2**
TOTAL	**CREDITS OF THE PROGRAMME**			
			CORE	**65**
			ELECTIVE	**7**
			PROJECT	**4**
			VIVA VOCE	**4**
			TOTAL CREDITS	**80**

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I

CH1CO1 - QUANTUM CHEMISTRY AND GROUP THEORY (3Credits, 54 hrs)

Unit 1: Introduction to Quantum Mechanics (9hrs)

Black body radiation and Planck's quantum postulate. Einstein's photoelectric equation, de Broglie's matter waves, Uncertainty principle, Schrodinger's wave mechanics, Deduction of Schrodinger wave equation from classical wave equation- Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, eigen functions of commuting operators; Expectation value postulate; Postulate of time dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((L_x, L_y, L_z), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.

Unit 2: Quantum Mechanics of Translational & Vibrational Motions (9hrs)

Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a one-dimensional box with one finite potential wall, Particle in a rectangular well, (no derivation), Significance of the problem, Introduction to tunneling; Particle in a three dimensional box, Separation of variables, degeneracy. Symmetry breaking.
One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, wave functions and energies, important features of the problem, harmonic oscillator model and molecular vibrations.

Unit: 3 Quantum Mechanics of Rotational Motion (9hrs)

Co-ordinate systems:- Cartesian, cylindrical polar and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution of the Phi-equation, One particle Rigid rotator (non planar rigid rotator or particle on a sphere) (complete treatment): Angular momentum in spherical polar co-ordinate, The wave equation in spherical polar coordinates, wave functions in the real form; separation of variables, the Phi-equation and the Theta-equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms),Converting imaginary functions to real form, polar diagrams of spherical harmonics. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2.

Unit 4: Quantum Mechanics of Hydrogen-like Atoms (9hrs)

Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots. angular functions (spherical harmonics) and their plots. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), spin orbitals, construction of spin orbitals fromorbitals and spin functions.

Unit 5: Foundations of Group Theory & Molecular Symmetry (9hrs)

Basic principles of group theory - the defining properties of mathematical groups, finite and infinite groups, Abelian and cyclic groups, group multiplication tables (GMT), similarity transformation, sub groups & classes in a group;
Molecular Symmetry & point groups - symmetry elements and symmetry operations in molecules, relations between symmetry operations, complete set of symmetry operations of a molecule, point groups and their systematic identification, GMT and classes of point groups;
Mathematical preliminaries - matrix algebra, addition and multiplication of matrices, inverse of a matrix, square matrix, character of a square matrix, diagonal matrix, direct product and direct sum of square matrices, block factored matrices, solving linear equations by the method of matrices;
Matrix representation of symmetry operations.

UNIT 6: Representations of Point Groups & Corresponding Theorems (9hrs)

Representations of point groups - basis for a representation, representations using vectors, atomic orbitals and cartesian coordinates positioned on the atoms of molecule (H_2O as example) as bases, reducible representations and irreducible representations (IR) of point groups, construction of IR by reduction (qualitative demonstration only), Great orthogonality theorem (GOT) (no derivation) and its consequences, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2V}, C_{3V}, C_{2h} and C_{4V} and C_3 as examples), nomenclature of IR - Mulliken symbols, symmetry species;
Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g., Γ_{cart}) using the reduction formula;
Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

Reference for **Units 1 to 4**

1. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,
3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition*, Pearson Education Inc., 2009.
4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
5. M.W. Hanna, *Quantum Mechanics in Chemistry* , 2nd Edition, W.A. Benjamin Inc., 1969.
6. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books,1983 (first Indian edition,Viva books, 2003).
7. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.
8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
9. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.
10. A.K. Chandra, *Introduction to Quantum Chemistry* , 4th Edition, Tata McGraw-Hill, 1994.
11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.

14. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
15. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry* , Prism Books Pvt. Ltd., 1998.
16. Jack Simons, *An Introduction to Theoretical Che mistry*, Cambridge University Press, 2003.

For Units 5&6

1. F.A. Cotton, *Chemical applications of Group Theory*, 3rd Edition, John Wiley &Sons Inc., 2003.
2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry*, John Wiley &Sons Inc., 1965.
3. L.H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill, 1969.
4. R. McWeeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London, 1963.
5. P.H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., New York, 1998.
6. Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood 1998.
7. A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry,* PHI Learning Pvt. Ltd. 2010.
8. Arthur M Lesk, *Introduction to Symmetry & Group theory for Chemists*, Kluwer Academicm Publishers,2004.
9. K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009.
10.A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I

CH1CO2 - ELEMENTS OF CHEMISTRY (3 Credits, 54hrs)

Unit 1: Molecular Structure and Bonding (9hrs)

The Lewis structure – Octet rule- Resonance – Formal charge –hypervalence-electroneutrality principle-Isoelectronic molecules. VSEPR theory, Walsh diagrams, dπ–pπ bonds. Bent rule, and energetics of hybridization. The hydrogen bond and its consequences-van der Waal`s forces-Determination of molecular structure by X-Ray diffraction.

Unit 2: Concepts of Acids and Bases (9hrs)

Major acid-base concepts, Arrhenius, Bronsted-Lowry, Solvent system, Lux-Flood, Lewis and Usanovich concepts. Classification of acids and bases as hard and soft. HSAB principle.-Theoretical basis of hardness and softness. The Drago-Wayland equation, E and C parameters-Symbiosis. Applications of HSAB concept. Chemistry of nonaqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4 and HSO_3 F. Nonaqueous solvents and acid-base strength. Super acids – surface acidity.

Unit 3: Chemistry of Main Group Elements-I (9hrs)

Chemical periodicity-First and Second raw anomalies-The diagonal relationship- Periodic anomalies of the nonmetals and post-transition metals.

Allotropes of C, S, P. As, Sb, Bi, O and Se. Electron deficient compounds-Boron hydrides-preparation, reactions, structure and bonding. Styx numberscloso,nido,arachno polyhedral structures. Boron cluster compounds-Wade’s rule. polyhedral borane anion-carboranes, metallaboranes and metallacarboranes. Borazines and borides.

Unit 4: Chemistry of Main Group Elements-II(9hrs)

Silicates and alumino silicates-Structure, molecular sieves-Zeolite.Silicones-Synthesis, structure and uses. Carbides and silicides. Synthesis, structure, bonding and uses of Phosphorous-Nitrogen, Phosphorous -Sulphur and Sulphur-Nitrogen compounds.

Unit 5: Chemistry of Transition and Inner Transition Elements (9hrs)

Heteropoly and isopoly anions of W, Mo, V.

Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram.

Differences between 4f and 5f orbitals. Magnetic and spectroscopic properties. Uranyl compounds. Trans-actinide elements. Super heavy elements –production and chemistry.

Unit 6: Nuclear and Radiation Chemistry (9hrs)

Structure of nucleus: shell, liquid drop, Fermi gas, collective and optical models. Nuclear reaction: Bethe`s notation of nuclear process- Types-reaction cross sectionphotonuclear

and thermonuclear reactions.
Nuclear fission: Theory of fission- neutron capture cross section and critical size.
Nuclear fusion. Neutron activation analysis
Radiation chemistry: Interaction of radiation with matter. Detection and measurement of radiation- GM and scintillation counters – radiolysis of water- radiation hazardsradiation dosimetry.

References

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements*, *2/e*, *Elsevier* Butterworth-Heinemann,2005.
2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi. *Inorganic Chemistry, principles of structure and reactivity,* Pearson Education, 2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry,* Pearson, 2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry,* Oxford University Press, 2002
5.William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press,2005.
6. Keith F Purcell, John C Kotz, *Inorganic Chemistry* , Cengage Learning, 2010.
7. James E House, *Inorganic Chemistry,* Academic Press, 2008.
8. H.J.Arnikar, *Essentials of Nuclear chemistry,* New Age International, 2005.
9. Friedlander and J.W.Kennedy, *Introduction to Radiochemistry,* John Wiley and Sons,1981.
10.S.Glastone, *Source Book on Atomic Energy, 3rd*edn., Affiliated East-West Press Pvt.Ltd., 1967.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I

CH1CO3 - STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS (3 Credits, 54hrs)

Unit 1: Structure and Bonding in Organic Molecules (9hrs)

Nature of Bonding in Organic Molecules: Localozed and delocalized Chemical Bonding, bonding weaker than covalent bond, Kinds of molecules with delocalized bond, cross-conjugation, resonance, rules of resonance, resonance hybrid and resonance energy, tautomerism, hyperconjugation, π-π interactions, pπ-dπ bonding (ylides).
Hydrogen bonding: Inter- and intramolecular hydrogen bonding. Range of the energy of hydrogen bonding. Effect of hydrogen bond on conformation, physical and chemical properties of organic compounds- volatility, acidity, basicity and stability. Stabilization of hydrates of glyoxal and chloral, and ninhydrin. High acid strength of maleic acid compared to fumaric acid. Electron donor-acceptor complexes, crown ether complexes, cryptates, inclusion compounds and cyclodextrins.
Hückel MO method. MO's of simple molecules, ethylene, allyl radical, 1,3-butadiene. Hückel rule and modern theory of aromaticity, criteria for aromaticity and antiaromaticity, MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes and heptalenes. Preparation of aromatic and antiaromatic compounds by different methods, stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.

Unit 2: Structure and Reactivity (9hrs)

Transition state theory, Potential energy vs Reaction co-ordinate curve, Substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity. Qualitative study of substitution effects in S_N1-S_N2 reactions. Neighbouring group participation, participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi - bond. Classical and nonclassical carbocations
Basic concepts in the study of organic reaction mechanisms: Application of Experimental criteria to mechanistic studies, Kinetic versus thermodynamic control- Hammond postulate, Bell-Evans-Polanyi principle, Marcus equation, Curtin-Hammet principles,.Acidity constant, Hammet acidity function.
Reactive intermediates and their characterizatin. Isotope effect (labeling experiments), stereochemical correlations. Semiquantitative study of substituent effects on the acidity of carboxylic acids. Quantitative correlation of substituent effects on reactivity. Linear free energy relationships. Hammet and Taft equation for polar effects and Taft's steric, substituent constant for steric effect. Solvent effects.

Unit 3: Conformational Analysis – I (9hrs)

Factors affecting the conformational stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformation of acyclic compounds – Ethane, nbutane, alkene dihalides, glycols, chlorohydrines, tartaric acid, erythro and threo isomer. Interconversion of axial and equatorial bonds in chair conformation of cylohexane – distance between the various H atoms and C atoms in chair and boat conformations. Monosubstituted cyclohexane – methyl and t-butyl cyclohexanes – flexible and rigid systems. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclohexanone, (cis & trans), 2-bromo-4,4- dimethyl cyclohexanone. Anchoring group and conformationaly biased molecules. Conformations of 1,4 cis and trans disubstituted cyclohexanes in which one of the substituent is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent. Conformations of decaline, adamentane, sucrose and lactose.

Unit 4: Conformational Analysis – II (9 hrs)

Effect of conformation on the course and rate of reactions in (a) Debromination of dl and meso 2,3 - dibromobutane or stilbene dibromide using KI. (b) Semipinacolic deamination of erythro and threo 1,2 -diphenyl-1-(p-chlorophenyl)-2-amino ethanol. (c) Dehydrohalogination of stilbene dihalide (dl and meso) and erythreo threo- bromo-1,2- diphenyl propane.

Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 reactions for (i) an axial substituent, and (ii) an equatorial substituent in flexible and rigid systems. (b) E1, E2 eliminations illustrated by the following compounds. (i) 4- t - Butylcyclohexyl tosylate (cis and trans) (ii) 2- Phenylcyclohexanol (cis and trans) (iii) Menthyl and neomenthyl chlorides and benzene hexachlorides. (c) Pyrolytic elimination of esters (cis elimination) (d) Esterification of axial as well as equatorial hydroxyl and hydrolysis of their esters in rigid and flexible systems. (Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol). (f) Esterification of axial as well as equatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorial tosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid. Bredt's rule. Stereochemistry of fused,, bridged and caged ring systems - decalins, norbornane, barrelene and adamantanes.

Unit 5: Stereochemistry (9hrs)

Conformation and configuration, Fischer, Newman and Sawhorse projection formulas and their interconversion. Concept of chirality, recognition of symmetry elements and chiral structures, conditions for optical activity, optical purity. Specific rotation and its variation in sign and magnitude under different conditions, relative and absolute configurations, Fisher projection formula, sequence rule – *R and S* notation in cyclic and acyclic compounds, Cahn-Ingold-Prelog (CIP) rule. Mixtures of stereoisomers; enantiomeric excess and diastereomeric excess and their determination. Methods of resolution diastereomers Resolution of racemates after conversion into diastereomers; use of Sbrucine, kinetic resolution of enantiomers, chiral chromatography.

Optical isomerism of compounds containing one or more asymmetric carbon atoms, enantiotopic, homotopic, diastereotopic hydrogen atoms, prochiral centre. Pro – R, Pro – S, Re and Si.

Optical isomerism in biphenyls, allenes and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Optical activity in cis-trans conformational isomers of 1,2-, 1,3- and 1,4-dimethylcyclohexanes .

Restricted rotation in biphenyls – Molecular overcrowding.

Chirality due to folding of helical structures.

Geometrical isomerism – E and Z notation of compounds with one and more double bonds in acyclic systems. Configuration of cyclic compounds-monocyclic, fused and bridged ring systems, inter conversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers in acyclic acid cyclic systems, stereochemistry of aldoximes and ketoximes

Unit 6: Asymmetric Synthesis (9 hrs)

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity and stereospecificity. Chiral pool: chiral pool synthesis of beetle pheromone component (*S*)- (–)-ipsenol from (S)-(–)-leucine.

Classification of Asymmetric reactions into (1) Substrate controlled (2) Chiral auxiliary controlled (3) Chiral reagent controlled and (4) Chiral catalyst controlled.

1. Substrate controlled asymmetric synthesis: Nucleophillic addition to chiral carbonyl compounds. 1,2 – asymmetric induction, Cram's rule and Felkin – Anh model.

2. Chiral auxiliary controlled asymmetric synthesis: α – Alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulfoxides. 1,4 – Asymmetric induction and Prelog's rule. Use of chiral auxiliary in Diels – Alder and Cope reactions.

3. Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL – H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$. Reduction with CBH reagent. Stereochemistry of Sharpless asymmetric epoxidation and dihydroxylation

4. Asymmetric aldol reaction: Diastereoselective aldol reaction and its explanation by Zimmermann – *Traxler* model. Auxillary controlled aldol reaction. Double diastereoselection – matched and mismatched aldol reactions.

References:

1. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A*, Springer, 5/e, 2007.
2. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, John Wiley & Sons, 6/e, 2007.
3. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press,2012.
5. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005.
6. M. S. Singh, *Advanced Organic Chemistry: Reactions and Mechanisms*, Pearson, 2013.
7. P. Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6/e, Pearson, 2006.
8. C. K. Ingold, Structure and Mechanism in Organic chemistry, 2/e, CBS Publishers, 1994.
9. E. L. Eliel, S. H. Wilen and L. N. Mander, *Stereochemistry of Carbon Compounds*, John Wiley, 1997.
10. G. L. D. Krupadanam, *Fundamentals of Asymmetric Synthesis*, Universities Press, 2013.
11. Okuyama and Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2013

12. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2/e, John Wiley & Sons, 2008.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I

CH1CO4 – THERMODYNAMICS, KINETICS AND CATALYSIS
(3 Credits, 54hrs)

Unit 1: Thermodynamics (9hrs)

Review of First and Second law of thermodynamics, Third law of thermodynamics, Need for third law, Nernst heat theorem, Apparent exceptions to third law, Applications of Third law, Determination of Absolute entropies, Residual entropy.
Thermodynamics of Solutions: Partial molar quantities, Chemocal potentioal, Variation of chemical potential with temperature and pressure, Partial molar volume and its determination, Gibbs-Duhem equation, Thermodynamics of ideal and real gases and gaseous mixtures, Fugacities of gases and their determinations, Activity, Activity coefficient, standard state of substance (for solute and solvents), Duhem-Margules equation and its applications. Thermodynamics of ideal solutions, Deduction of the laws of Raoult's ebullioscopy, cryoscopy, and osmotic pressure. Non ideal solutions, Deviations from Raoult's law, Excess functions-excess free energy, excess entropy, excess enthalpy, excess volume.

Unit 2: Thermodynamics of Irreversible Processes (9 hrs).

Simple examples of irreversible processes, general theory of non –equilibrium processes, entropy production, the phenomenological relations, Onsager reciprocal relations, application to the theory of diffusion, thermal diffusion, thermo-osmosis and thermo-molecular pressure difference, electro-kinetic effects, the Glansdorf –Pregogine equation.

Unit 3: Chemical Kinetics (9 hrs)

Kinetics of reactions involving reactive atoms and free radicals - Rice – Herzfeld mechanism and steady state approximation in the kinetics of organic gas phase decompositions (acetaldehyde & ethane); Kinetics of chain reactions – branching chain and explosion limits (H_2-O_2 reaction as an example); Kinetics of fast reactionsrelaxation methods, molecular beams, flash photolysis; Solution kinetics: Factors affecting reaction rates in solution, Effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects.

Unit 4: Molecular Reaction Dynamics (9 hrs)

Reactive encounters: Collision theory, diffusion controlled reactions, the material balance equation, Activated Complex theory – the Eyring equation, thermodynamic aspects of ACT; Comparison of collision and activated complex theories; The dynamics of molecular collisions – Molecular beams, principle of crossed-molecular beams; Potential energy surfaces - attractive and repulsive surfaces, London equation, Statistical distribution of molecular energies; Theories of unimolecular reactions - Lindemann's theory, Hinshelwood's modification, Rice -Ramsperger and Kassel (RRK) model.

Unit 5: Surface Chemistry (9 hrs)

Adsorption: Adsorption isotherms, Langmuir's unimolecular theory of adsorption, BET equation, derivation, determination of surface area of adsorbents, heat of adsorption and its determination; Experimental methods for studying surfaces – SEM, TEM, and ESCA.

Unit 6: Catalysis (9hrs)

Homogeneous catalysis – mechanism -Arrhenius intermediates and van't Hoff intermediates - acid base catalysis – specific and general acid catalysis – enzyme catalysis- Michaelis-Menten Mechanism- Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko - Volterra, brusselator and oregonator) Heterogenous catalysis –adsorption and catalysis- unimolecular surface reactions – bimolecular surface reaction –Langmuir-Hinshelwood echanism and Eley-Rideal mechanism – illustration using the reaction $2CO + O_2$. $2CO_2$

References:

1. *P. Atkins & J. De Paula, Atkins's Physical Chemistry, 10/e, OUP, 2014*.
2 Keith J. Laidler, *Chemical Kinetics 3rd edn*., Pearson Education, 1987(Indian reprint 2008).
3. Steinfeld, Francisco and Hase, *Chemical Kinetics and Dynamics 2 nd edition*, Prentice Hall International . Inc
4. Santhosh K. Upadhyay, *Chemical Kinetics and Reaction Dynamics,* Springer, 2006.
5. Richard I. Masel, *Chemical Kinetics and Catalysis* , Wiley Interscience, 2001.
6. K.J.Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.
7. A.W. Adamson, *Physical Chemistry of surfaces* , 4th edition, Interscience, New York, 1982.
8. G. K. Vemulapalli, *Physical Chemistry,* Printice Hall of India.
9. M.K. Adam, *The Physics and Chemistry of surfaces* , Dover Publications
10. S. Glasstone, *Thermodynamics for chemists,* East-West 1973.
11. Rajaram and Kuriokose, *Thermodynamics,* East-West 1986
12. Pigoggine, *An introduction to Thermodynamics of irreversible processes* , Interscience
13. B.G. Kyle, *Chemical and Process Thermodynamics*, 2nd Edn, Prentice Hall of India

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II

CH2CO5 - APPLICATIONS OF QUANTUM MECHANICS AND GROUP THEORY (3 Credits, 54hrs)

Unit 1: Approximation Methods in Quantum Mechanics (9hrs)

Many body problem and the need of approximation methods; Independent particlemodel; Variation method – variation theorem with proof, illustration of variationtheorem using a trial function [e.g., x (a-x)] for particle in a 1D-box and using the trialfunction $e^{-\alpha r^2}$ for the hydrogen atom, variation treatment for the ground state of heliumatom; Perturbation method – time-independent perturbation method (non-degeneratecase only), illustration by application to particle in a ID-box with slanted bottom,perturbation treatment of the ground state of the helium atom.

Unit 2: Quantum Mechanics of Many-electron Atoms (9hrs)

Hartree Self-Consistent Field method for atoms; Spin orbitals for many electron atoms,symmetric and antisymmetric wave functions, Pauli's antisymmetry principle; Slater determinants; Hartree -Fock Self- Consistent Field (HF-SCF) method for atoms, Hartree-Fock equations (derivation not required) & the Fock operator; Roothan's concept of basis functions – Slater type orbitals (STO) and Gaussian type orbitals (GTO).

Unit 3: Chemical bonding in diatomic molecule (9hrs)

Schrödinger equation for a molecule, Born – Oppenheimer approximation; Valence Bond (VB) theory – VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2; Molecular Orbital (MO) theory – MO theory of H2 + ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules – Li_2, Be_2, C_2, N_2, O_2 & F_2 and hetero nuclear diatomic molecules – LiH, CO, NO & HF, bond order, correlation diagrams, non-crossing rule; Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories.

Unit 4: Chemical Bonding in polyatomic molecules (9hrs)

Hybridization – quantum mechanical treatment of sp, sp^2 & sp^3 hybridisation; Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion, charge distributions and bond orders from the coefficients of HMO, calculation of free valence, HMO theory of aromatic hydrocarbons (benzene); formula for the roots of the Hückel determinantal equation, Frost -Hückel circle mnemonic device for cyclic polyenes.

Unit 5: Applications of Group Theory to Molecular Spectroscopy (9hrs)

Molecular vibrations - symmetry species of normal modes of vibration, construction of Tcart, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra.

Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non –vanishing integrals, transition moment integral and spectral transition probabilities, overlap integrals and conditions for overlap. Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

Unit 6: Applications of Group Theory to Chemical Bonding (9hrs)

Hybridisation - Treatment of hybridization in BF_3 and CH_4, Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – HCHO and H_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using proj ection operator, use of projection operator in constructing SALCs for the π MOs in cyclopropenyl ($C_3H_3^{+}$) cation.

References (for Units 1 to 4)

1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry,* 6th Edition, Pearson Education Inc.,
3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition,* Pearson Education Inc., 2009.
4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 4th Edition, Oxford University Press, 2005.
5. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc.,1969.
6. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition, Viva books, 2003).
7. Thomas Engel, *Quantum Chemistry & Spectroscopy,* Pearson Education, 2006.
8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
9. Horia Metiu, *Physical Chemistry–Quantum Mechanics*, Taylor & Francis, 2006.
10. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw-Hill, 1994.
11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics,* McGraw-Hill, 1935 (A good source book for many derivations).
12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
14. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
15. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd.,1998.
16. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003

For Units 5&6

1. F.A.Cotton, *Chemical applications of Group Theory*, 3rd Edition, John Wiley &Sons Inc. 2003.

2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry,* John Wiley &Sons Inc., 1965.
3 .L.H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill, 1969.
4.R. McWeeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London, 1963.
5. P.H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., NewYork, 1998.
6. Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood 1998.
7. A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry,* PHI Learning Pvt. Ltd. 2010.
8. Arthur M Lesk, *Introduction to Symmetry & Group theory for Chemists*, Kluwer Academic Publishers, 2004.
9. K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009.
10. A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers, 1997.

CH2CO6 - CO-ORDINATION CHEMISTRY (3Credits, 54hrs)

Unit 1: Stability of Co-ordination Compounds (9hrs)

Stereochemistry of coordination compounds. Stepwise and overall formation constants and the relationship between them. Trends in stepwise formation constants.Determination of binary formation constants by pH-metry and spectrophotometry.Stabilisation of unusual oxidation states. Ambidentate and macrocyclic ligands. Chelate effect and its thermodynamic origin. Macrocyclic and template effects.

Unit 2: Theories of Bonding in Coordination Compounds (9hrs)
Sidgwick`s electronic interpretation of coordination. The valence bond theory and its limitations. The crystal field and ligand field theories. Splitting of d-orbitals in octahedral, tetrahedral and square planar fields. Factors affecting crystal field splitting. Spectrochemical and nephelauxetic series. Racah parameters. Jahn-Teller effect. Molecular orbital theory-composition of ligand group orbitals. MO diagram of octahedral, tetrahedral and square planar complexes. π-bonding and molecular orbital theory.

Unit 3: Electronic Spectra and Magnetic Properties of Complexes (9hrs)

Spectroscopic ground state. Terms of dn configurations. Selection rules for d-d transitions. Effect of ligand fields on RS terms in octahedral and tetrahedral complexes. Orgel diagrams. Calculation of Dq, B and β parameters. Tanabe-Sugano diagrams. Charge transfer spectra.

Types of magnetic properties-Paramagnetism and diamagnetism. Curie and Curie-Weiss laws.The μ_J , μ_{L+S} , and μ_S expressions. Orbital contribution to magnetic moment and its quenching. Spin-orbit coupling. Temperature independent paramagnetism. Antiferromagnetism-types and exchange pathways. Determination of magnetic moment by Gouy method.

Unit 4: Characterization of Coordination Complexes (9hrs)

Infrared spectra of metal complexes. Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Application in coordination complexes. ESR spectra – application to copper complexes. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling. Mossbauer spectroscopy- the Mossbauer effect, hyperfine interactions (qualitative treatment). Application to iron and tin compounds.

Unit 5: Reaction Mechanism of Metal Complexes (9hrs)

Ligand substitution reactions. Labile and inert complexes. Rate laws. Classification of mechanisms-D, A and I mechanisms. Substitution reactions in octahedral complexes. The Eigen-Wilkins Mechanism. Fuoss-Eigen equation. Aquation and base hydrolysismechanism.

Substitution reactions in square planar complexes. The trans effect-Applications and theories of trans effect. The cis effect.

Unit 6: Redox and Photochemical Reactions of Complexes (9hrs)

Classification of redox reaction mechanisms. Outer sphere and inner sphere mechanisms. Marcus equation. Effect of the bridging ligand. Methods for distinguishing outer- and inner-sphere redox reactions.

Photochemical reactions of metal complexes- Prompt and delayed reactions. Exited states of metal complexes- Interligand, ligand field, charge transfer and delocalized states. Properties of ligand field excited states. Photosubstitution-Prediction of substitution lability by Adamson`s rules. Photoaquation. Photo isomerisation and photo recimization. Illustration of reducing and oxidizing character of $[Ru(bipy)_3]^{2+}$ in the excited state. Metal complex sensitizers- water photolysis.

References:

1. N.N.Greenwood and A.Earnshaw, *Chemistry of Elements, 2/e,* Butterworth- Heinemann, 2005.
2 J.E.Huheey, E.A.Keiter, R.L.Keiter and O.K.Medhi, *Inorganic Chemistry, principles of structure* and *reactivity*, Pearson Education, 2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry,*Pearson, 2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry,*Oxford University Press, 2002
5. William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press, 2005.
6 .Keith F Purcell, John C Kotz, *Inorganic Chemistry*, Cengage Learning, 2010.
7. James E House, *Inorganic Chemistry,* Academic Press, 2008.
8. B.Douglas, D.McDaniel, J.Alexander, *Concepts and Models of Inorganic Chemistry,*Wiley Student Edition, 2006.
9. A.W.Adamson and P.D.Fleischauer, *Concepts of Inorganic Photochemistry, Wiley.*
10. F.A.Cotton and G.Wilkinson, *Advanced Inorganic Chemistry*, Wiley.
11. A.Earnshaw, *Introduction to Magnetochemistry, Academic Press, 1968.*
12. R.L.Dutta and A.Shyamal, *Elements of Magnetochemistry,* S.Chand and Co. 1982.
13. A.E. Martell, *Coordination Chemistry, Vol. I*
14. R.S. Drago, *Physical Methods in Inorganic Chemistry*, Affiliated East- West Press Pvt. Ltd., 1977

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II

CH2CO7 - REACTION MECHANISM IN ORGANIC CHEMISTRY(3 Credits, 54hrs)

Unit 1: Aliphatic and Aromatic Substitutions (9 hrs)

Nucleophilic Aliphatic Substitution: Mechanism and Stereochemistry of S_N2 and S_N1 reactions. Ion pair mechanism. The effect of substrate structure, reaction medium, nature of leaving group and nucleophile on S_N2 and S_N1 reactions. S_Ni and neighboring group mechanism. SET mechanism. Allylic and bezylic substitutions. Ambident nucleophiles and substrates regioselectivity.

Electrophilic Aliphatic Substitution: Mechanism and stereochemistry of S_E1, S_E2 (front), S_E2 (back) and S_Ei reactions. The effect of substrate structure, leaving group and reaction medium on S_E1 and S_E2 reactions.

Electrophilic Aromatic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity. Nucleophilic Aromatic substitution: Addition-elimination (S_NAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, S_N1 and $S_{RN}1$ mechanism. The effect of substrate structure, nucleophile and leaving group on aromatic Nucleophilic substitution.

Unit 2: Addition & Elimination Reactions and Reactive Intermediates (9hrs)

(i) Addition and Elimination Reactions (6 hrs)
Mechanistic and stereochemical aspects of addition to C=C involving electrophiles, nucleophiles and free radicals. Effect of substituents on rate of addition, orientation of addition, addition to conjugated systems and cyclopropane rings, Michael reaction.

Mechanistic and stereochemical aspects of E1, E1cB and E2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev *vs* Hofmann elimination, α-elimination, pyrolytic *syn* elimination (E*i*) and conjugate eliminations. Competition between substitution and elimination reactions, basicity *vs* nucleophilicity. Extrusion reactions-extrusion of N_2, CO and CO_2.

(ii) Reactive Intermediates (3 hrs)
Reactive Intermediates: Generation, geometry, stability and reactions of carbonium ions and carbanions, free radicals, carbenes, nitrenes and benzynes.

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

(i) Reactions of Carbon-heteromultiple Bonds (7 hrs)
Reactivity of carbonyl compounds toward addition, mechanistic aspects of hydration, addition of alcohols, and condensation with nitrogen nucleophiles to aldehydes and ketones. Addition of organometallic reagents- Grignard reagents- organozinc, organocopper and organolithium

reagents- to carbonyl compounds. Aldol, Perkin, Claison, Dieckmann, Stobbe and benzoin condensation. Darzen's, Knoevenagel, Reformatsky, Wittig, Cannizaro, Mannich and Prins reactions. MPV reduction and Oppenauer oxidation. Addition to carbon-nitrogen multiple bond: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis and reduction of nitriles.

(ii) Esterification and Ester Hydrolysis (2hrs): Mechanisms of ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.

Unit 4: Pericyclic Reactions (9 hrs)

Phase and symmetry of molecular orbitals, FMOs of ethylene, 1,3-butadiene, 1,3,5- hexatriene, allyl and 1,3-pentadienyl systems. Pericyclic reactions: electrocyclic, cycloaddition, sigmatropic, chelotropic and group transfer reactions. Theoretical models of pericyclic reactions: TS aromaticity method (Dewar-Zimmerman approach), FMO method and Correlation diagram method (Woodward-Hoffmann approach). Woodward- Hoffmann selection rules for electrocyclic, cycloaddition and sigmatropic reactions. Stereochemistry of Diels-Alder reactions and regioselectivity. Cope and Claison rearrangements. Stereochemistry of cope rearrangement and valence tautomerism. 1,3- dipolar cycloaddition reactions and *ene* reactions.

Unit 5: Photochemistry of Organic Compounds (9 hrs)

Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization and quenching. Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and β, γ-unsaturated carbonyl compounds, β- cleavage, γ- hydrogen abstraction: Norrish type-II cleavage, photo reduction, photoenolization. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Büchi reaction, photodimerisation of α, β-unsaturated ketones, Photo rearrangemets: Photo–Fries, di-π- methane, lumiketone, oxa di-π-methane rearrangements. Barton and Hoffmann-Loeffler Freytag reactions. Photo isomerisation and dimerisation of alkenes, photo isomerisation of benzene and substituted benzenes, photooxygenation.

Unit 6: Chemistry of Natural Products (9 h)

Chemical classification of natural products. Classification of alkaloids based on ring structure, isolation and general methods of structure elucidation based on degradative reactions. Structures of atropine and quinine. Terpenoids - Isolation and classification of terpenoids, structure of steroids classification of steroids. Woodward synthesis of cholesterol, conversion of cholesterol to testosterone. Total synthesis of Longifolene, Reserpine, Cephalosporin, Introduction to flavonoids and anthocyanins (Structures only)

References:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
2. F. A. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, *Part A & B*, 5/e, Springer, 2007.

3. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005.
4. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.
5. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3/e, CRC Press, 1998.
6. Peter Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6/e, Pearson, 2006.
7. S. Sankararaman, *Pericyclic Reactions-A Textbook: Reactions, Applications and Theory*, Wiley VCH, 2005.
8. I. Fleming, *Molecular Orbitals and Organic Chemical Reactions*, Wiley, 2009.
9. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age International, 2012.
10. G. M. Loudon, *Organic Chemistry,* 4/e, Oxford University Press, 2008
11. M. B. Smith, *Organic Chemistry: An Acid Base Approach*, CRC Press, 2010.
12. T. Okuyama and H. Maskill, *Organic Chemistry A Mechanistic Approach*, Oxford University Press, 2014.
13. I. Fleming, *Selected Organic Synthesis*, John Wiley and Sons, 1982.
14. T. Landbery, *Strategies and Tactics in Organic Synthesis*, Academic Press, London,1989.
15. E. Corey and I.M. Chang, *Logic of Chemical Synthesis*, John Wiley, New York, 1989.
16. I. L. Finar, *Organic Chemistry Vol 2: Stereochemistry and the Chemistry of Natural Products*, 5/e, Pearson, 2006.
17. N. R.Krishnaswamy, *Chemistry of Natural Products: A Laboratory Hand Book*, 2/e, Universities Press

MSc. CHEMISTRY (CSS PATTERN) - SEMESTER II

CH2CO8 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS (3 Credits, 54hrs)

Unit 1: Ionic Interaction & Equilibrium Electrochemistry (9hrs)

The nature of electrolytes, Ion activity, Ion-ion and ion-solvent interaction, The electrical potential in the vicinity of an ion, Electrical potential and thermodynamic functions. The Debye-Hückel equation,Limiting and extended forms of the Debye- Hückel equation, Applications of the Debye Hückel equation for the determination of thermodynamic equilibrium constants and to calculate the effect of ionic strength on ion reaction rates in solution

Origin of electrode potentials-half cell potential-standard hydrogen electrode, reference electrodes-electrochemical series, applications- cell potential, Nernst equation for electrode and cell potentials, Nernst equation for potential of hydrogen electrode and oxygen electrode- thermodynamics of electrochemical cells, efficiency of electrochemical cells and comparison with heat engines-primary cells (Zn, MnO_2) and secondary cells (lead acid, Ni-Cd and Ni-MH cells), electrode reactions, potentials and cell voltages, advantages and limitations three types of secondary cells. -fuel cells; polymer electrolyte fuel cell (PEMFCs), alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), direct methanol fuel cells, electrode reactions and potentials, cell reactions and cell voltages, advantages and limitations of four types of fuel cells

Unit 2: Dynamic Electrochemistry (9hrs)

Electrical double layer-electrode kinetics of electrode processes, the Butler-Volmer equation-The relationship between current density and overvoltage, the Tafel equation. Polarization - electrolytic polarization, dissolution and deposition potentials, concentration polarization; Overvoltage: hydrogen overvoltage and oxygen overvoltage: decomposition potential and overvoltage, individual electrode over voltages and its determination-metal deposition over voltage and its determination- theories of hydrogen overvoltage, the catalytic theory, the slow discharge theory, the electrochemical theory.
Principles of polarography -dropping mercury electrode, the half wave potential.

UNIT 3: Solid State – I (9hrs)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies & Hermann–Mauguin notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups.

Bragg's law and applications, lattice planes and miller indices, *d*-spacing formulae, crystal densities and unit cell contents,
Imperfections in solids - point, line and plane defects, non-stoichiometry.

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UNIT 4: Solid State – II (9hrs)

Electronic structure of solids – free electron theory, band theory & Zone theory, Brillouin zones; Electrical properties - electrical conductivity, Hall effect, dielectric properties, piezo electricity, ferro-electricity and ionic conductivity; Superconductivity- Meissner effect, brief discussion of Cooper theory of superconductivity; Optical properties - photo conductivity, luminescence, colour centers, lasers, refraction & birefringence; Magnetic properties - diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagnetism; Thermal properties - thermal conductivity & specific heat

Unit 5: Statistical Thermodynamics- I (9hrs)

Fundamentals – concept of distribution, thermodynamic probability and most probable distribution, ensembles, statistical mechanics for systems of independent particles and its importance in chemistry, thermodynamic probability & entropy, idea of microstates and macrostates, statistical weight factor (g), Sterling approximation, Maxwell- Boltzman statistics. The molecular partition function and its relation to the thermodynamic properties, derivation of third law of thermodynamics, equilibriumconstant & equi-partition principle in terms of partition functions, relation between molecular & molar partition functions, factorisation of the molecular partition function into translational, rotational, vibrational and electronic parts, the corresponding contributions to the thermodynamic properties; Evaluation of partition functions and thermodynamic properties for ideal mono-atomic and diatomic gases.

Unit 6: Statistical Thermodynamics- II (9hrs)

Heat capacities of solids - classical and quantum theories, Einstein's theory of atomic crystals and Debye's modification. Quantum Statistics: Bose - Einstein distribution law, Bose-Einstein condensation, application to liquid helium; Fermi - Dirac distribution law, application to electrons inmetals; Relationship between Maxwell-Boltzman, Bose-Einstein, and Fermi-Dirac statistics.

References:

For Units 1-4

1. D. R. Crow, *Principles and Applications of Electrochemistry*, Chapman and Hall London, 1979.
2. J.O.M. Bockris and A.K.N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic / Plenum Publishers, 2000.
3. Carl. H. Hamann, A. Hamnett, W.Vielstich, *Electrochemistry 2nd edn*., Wiley- VCH, 2007.
4. Philip H Reiger, *Electrochemistry 2nd edn*., Chapman & Hall, 1994.
5. Praveen Tyagi, *Electrochemistry,* Discovery Publishing House, 2006.
6. D.A. McInnes, *The Principles of Electrochemistry*, Dover publications, 1961.
7. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY, 1960.
8. A.R. West, *Basic Solid State Chemistry 2nd edn.*, John Wiley & Sons, 1999.
3. A.R. West, *Solid State Chemistry & its Applications,* John Wiley & Sons, 2003 (Reprint 2007).
4. Charles Kittel, *Introduction to Solid State Physics, 7th edn*, John Wiley & Sons, 2004 (Reprint 2009).
5. Mark Ladd, *Crystal Structures: Lattices & Solids in Stereo view*, Horwood, 1999.
6. Richard Tilley, *Crystals & Crystal Structures*, John Wiley & Sons, 2006.
7. C. Giacovazzo (ed.) *Fundamentals of Crystallography 2nd edn.*, Oxford Uty. Press, 2002.
8. Werner Massa, *Crystal Structure Determination 2nd edn*., Springer 2004.

9. N.B. Hanna, *Solid state Chemistry*, Prentice Hall

For Units 5 & 6

1. G.S. Rush Brooke, *Statistical mechanics,* Oxford University Press.
2. T.L. Hill, *Introduction to statistical thermodynamics*, Addison Wesley.
3. K. Huary, *Statistical mechanics, Thermodynamics and Kinetics* , John Wiley.
4. O.K.Rice, *Statistical mechanics, Thermodynamics and Kinetics*, Freeman and Co.
5. F.C. Andrews, *Equilibrium statistical mechanics* , John Wiley and sons, 1963.
6. M.C. Guptha, *Statistical Thermodynamics* , Wiley eastern Ltd., 1993.

M.Sc. CHEMISTRY – SEMESTER I & II

CH1PO1 & CH2PO4 – INORGANIC CHEMISTRY PRACTICALS– I & II
(4 Credits)

UNIT 1: Inorganic Cation Mixture Analysis
Separation and identification of four metal ions of which two are less familiar elements like W, Se Te, Mo, Ce, Th, Ti, Zr, V, U and Li. (Eliminating acid radicals not present). Confirmation by spot tests.

UNIT 2: Volumetric Analysis
Volumetric Determinations using:
(a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)
(b) Cerimetry (Fe^{2+},nitrite)
(c) Potassium Iodate (Iodide, Sn^{2+})

UNIT 3: Colorimetric Analysis
Colorimetric Determinations of metal ions Fe, Cr, Ni, Mn and Ti.

References
1. G.H. Jeffery, J. Basseett, J. Mendham and R.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edition, ELBS, 1989.
2. D.A. Skoog and D.M. West, *Analytical Chemistry, An Introduction*, 4th Edition, CBS Publishing Japan Ltd., 1986.
3. E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, *Quantitative Chemical Analysis*, 4th Edition, The Macmillan Company, 1969.
4. R.A. Day (Jr.) and A.L. Underwood, *Quantitative Analysis*, 6th Edition, Prentice Hall of India, 1993.

M.Sc. CHEMISTRY – SEMESTER I & II

CH1PO2 & CH2PO5 – ORGANIC CHEMISTRY PRACTICALS– I & II
(4 Credits)

Unit 1: Laboratory Techniques

Methods of Separation and Purification of Organic Compounds – fractional, steam and low-pressure distillations, fractional crystallisation and sublimation.

Unit 2: Separation and identification of the components of organic binary mixtures. (Microscale analysis is preferred)

Analysis of about ten binary mixtures, some of which containing compounds with more than one functional group. Separation and identification of a few ternary mixtures.

Unit 3: Organic preparations-double stage (minimum six) and three stage (minimum two)

References:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5/e, Pearson, 1989.
2. Shriner, Fuson and Cartin, *Systematic Identification of Organic Compounds*, 1964.
3. Fieser, *Experiments in Organic Chemistry*, 1957.
4. Dey, Sitaraman and Govindachari, *A Laboratory Manual of Organic Chemistry*, 3rdEdition, 1957.
5. P.R. Singh, D.C. Gupta and K.S. Bajpal, *Experimental Organic Chemistry*, Vol. I and II, 1980.
6. Vishnoi, *Practical Organic Chemistry*.
7. Pavia, Kriz, Lampman, and Engel, *A Microscale Approach to Organic Laboratory Techniques*, 5/e, Cengage, 2013.
8. Mohrig, Hammond and Schatz, *Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale*, 3/e, W. H. Freeman and Co., 2010.

M.Sc. CHEMISTRY – SEMESTER I & II

CH1PO3 & CH2PO6 – PHYSICAL CHEMISTRY – I & II (4 Credits)

SECTION A

Unit 1: Solubility and Heat of solution (minimum 2 experiments)
1. Determination of molar heat of solution of a substance (e.g., ammonium oxalate, succinic acid) from solubility data - analytical method and graphical method

Unit 2: Phase Equilibria (minimum 3 experiments)
1. (a) Determination of phase diagram of a simple eutectic system (e.g., Biphenyl, Naphthalene-Diphenyl amine) (b) Determination of the composition of a binary solid mixture.
2. Determination of phase diagram of a binary solid system forming a compound (e.g., Naphthalene – m-dinitrobenzene).

Unit 3: Viscosity (minimum 2 experiments)
1. Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene - nitrobenzene, water-alcohol).
2. Determination of molecular weight of a polymer (e.g., polystyrene in

Unit 4: Distribution Law (minimum 3 experiments)
1. Determination of distribution coefficient of I_2 between CCl_4 and H_2O.
2. Determination of equilibrium constant of $KI + I_2 = KI_3$
3. Determination of concentration of KI solution

SECTION B

Unit 5: Refractometry (minimum 3 experiments)
1. Determination of molar refractions of pure liquids (e.g., water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol)
2. Determination of composition of liquid mixtures (e.g., alcohol -water, glycerol-water)
3. Determination of molar refraction and refractive index of a sol id

Unit 6: Conductivity (minimum 4 experiments)
1. Determination of equivalent conductance of a weak electrolyte (e.g., acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.
2. Determination of solubility product of a sparingly soluble salt (e.g., AgCl, $BaSO_4$)
3. Conductometric titrations
(a) HCl vs NaOH
(b) (HCl + CH_3-COOH) vs NaOH
4. Determination of the degree of hydrolysis of aniline hydrochloride

Unit 7: Potentiometry (minimum 3 experiments)

1. Potentiometric titration: HCl vs NaOH, CH_3-COOH vs NaOH
2. Redox titration: KI vs $KMnO_4$, $FeSO_4$ vs $K_2Cr_2O_7$
3. Determination of dissociation constant of acetic acid by potentiometric titration
4. Determination of pH of weak acid using Potentiometry
5. Determination of pH of acids and bases using pH meter

References:

1. A. Finlay, *Practical Physical Chemistry*, Longman's Green & Co.
2. J.B. Firth, *Practical Physical Chemistry*, Read Books (Reprint 2008).
3. A.M. James, *Practical Physical Chemistry*, Longman, 1974.
4. F. Daniel, J.W. Williams, P. Bender, R.A. Alberty, C.D. Cornwell and J.E. Harriman, *Experimental Physical Chemistry* , McGraw Hill, 1970.
5. W.G. Palmer, *Experimental Physical Chemistry*, 2nd Edition, Cambridge University Press, 1962.
6. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry*, McGraw Hill.
7. J. B. Yadav, *Advanced Practical Physical Chemistry, Goel Publications*, 1989.
8. B. Viswanathan & R.S. Raghavan, *Practical Physical Chemistry*, Viva Books, 2009

CH3CO9 - MOLECULAR SPECTROSCOPY (3 Credits, 54hrs)

Unit1: Basic Aspects and Microwave Spectroscopy - *Theory only* (9hrs)

Electromagnetic radiation & it's different regions, Interaction of matter with radiation and its effect on the energy of a molecule, Factors affecting the width and Intensity of Spectral lines-

Microwave spectroscopy - Rotation spectra of diatomic and poly atomic molecules - rigid and non-rigid rotator models, asymmetric, symmetric and spherical tops, isotope effect on rotation spectra, Stark effect, nuclear and electron spin interactions, rotational transitions and selection rules, determination of bond length using microwave spectral data.

Unit 2: Infrared and Raman Spectroscopy - (9hrs)

Vibrational spectroscopy -Normal modes of vibration of a molecule; Vibrational spectra of diatomic molecules, anharmonicity, Morse potential, fundamentals, overtones, hot bands, combination bands, difference bands; Vibrational spectra of polyatomic molecules; Vibrationrotation spectra of diatomic and polyatomic molecules, spectral branches -P, Q & R branches.

Infrared Spectroscopy: Functional group and finger print regions, Factors affecting vibrational frequency: Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding. Important absorption frequencies of different class of organic compounds- hydrocarbons, alcohols, thiols, carbonyl compounds, amines, nitriles

Raman spectroscopy –Classical and Quantum theory of Raman effect Pure rotational & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle; Introduction to Resonance Raman spectroscopy (basics only).

Unit 3: Magnetic Resonance Spectroscopy - *Theory only* (9hrs)

NMR: Quantum mechanical description of Energy levels-Population of energy-Transition probabilities using ladder operators-Nuclear shielding- Chemical shift- Spin-Spin coupling and splitting of NMR signals- Quantum mechanical Description- AX and AB NMR pattern-Effect of Relative magnitudes of J (Spin-Spin coupling) and Chemical Shift on the spectrum of AB type molecule. Karplus relationship.- Nuclear Overhauser Effect- FT NMR- Pulse sequence for T1 and T2 (Relaxation) measurements. 2D NMR COSY

Electron Spin Resonance: Quantum mechanical description of electron spin in a magnetic field- Energy levels-Population- Transition probabilities using Ladder operators- g factor-hyperfine interaction-Mc Connell Relation-Equivalent and non equivalent nucleus- g anisotropy- Zero field splitting -Kramer's theorem.

Mossbauer Spectroscopy: The Mossbauer effect, hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfine interactions.

UNIT 4: Electronic Spectroscopy (9hrs)

Electronic Spectroscopy- Characteristics of electronic transitions – Vibrational coarse structure, intensity of electronic transitions, Franck - Condon principle, types of electronic transitions; Dissociation and pre-dissociation; Ground and excited electronic states of diatomic molecules; Electronic spectra of polyatomic molecules; Electronic spectra of conjugated molecules;

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating **λmax** of dienes, enones and benzene derivatives.

Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights, circular birefringence, elipticity and circular dichroism, ORD and Cotton effect. Octant rule and Axial haloketone rule for the determination of conformation and configuration of 3-methyl cyclohexanone and *cis*- and *trans*-decalones. CD curves.

UNIT 5: NMR Spectroscopy in Organic Chemistry (9hrs)

^{1}HNMR: Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values of protons in common organic compounds, Chemical, magnetic and stereochemical equivalence. Enantiotopic, daisteriotopic and homotopic protons. Protons on oxygen and nitrogen. Quadrapole broadening. Spin –spin coupling, types of coupling. Coupling constant, factors influencing coupling constant, effects of chemical exchange, fluxional molecules, hindered rotation on NMR spectrum, First order and non first order nmr spectra, Simplification of NMR spectra: double resonance, shift reagents, increased field strength, deuterium labelling. NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra.

^{13}CNMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls,

and aromatics. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.

UNIT 6: Mass Spectrometry and Spectroscopy for Structure Elucidation (9hrs)

Mass Spectrometry: Basic concept of EIMS. Molecular ion and meta stable ion peaks, Isotopic peaks. Molecular weight and molecular formula. Single and multiple bond cleavage, rearrangements -McLafferty rearrangements. Fragmentation pattern of some common organic compounds – saturated and unsaturated hydrocarbons, ethers, alcohols, aldehydes and ketones, amines and amides. High resolution mass spectrometry, index of hydrogen deficiency, Nitrogen rule and Rule of Thirteen. Ionization techniques. FAB spectra.

Structural determination of organic compounds using spectroscopic techniques (Problem solving approach)

References: For Units 1, 2 & 3:

1. G.M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.

2. C.N. Banwell & E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill,New Delhi, 1994.

3. Thomas Engel, *Quantum Chemistry & Spectroscopy*, Pearson education, 2006.

4. P. Atkins & J. De Paula, *Atkins's Physical Chemistry,* 8th Edition, W.H. Freeman & Co., 2006.

5. D.A. McQuarrie and J.D. Simon, *Physical Chemistry - A Molecular Approach*, University Science Books, 1997.

6. D.N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, UniversityPress, 2000.

7. R.S. Drago, *Physical methods for Chemists*, Second edition, Saunders College Publishing 1977 (For NMR and EPR, Mossbauer)

8. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 2/e, – John Wiley

9. Ferraro, Nakamoto and Brown, Introductory Raman Spectroscopy, 2/e, Academic Press, 2005.

For Units 4, 5 & 6

1. Lambert, Organic Structural Spectroscopy, 2/e,—Pearson

2. Silverstein, Spectrometric Identification of Organic Compounds, 6/e,—John Wiley

3. Pavia, Spectroscopy, 4/e, – Cengage

4. Jag Mohan, Organic Spectroscopy: Principles and Applications, 2/e,—Narosa

5. Fleming, Spectroscopic Methods in Organic Chemistry, 6/e, — McGraw-Hill

6. P S Kalsi, Spectroscopy of organic compounds, New Age International, 2007

7. William Kemp, Organic Spectroscopy**, 3e,** Palgrave, 2010

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

CH3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY (3Credits, 54h)

Unit 1: Introduction to Organometallic Chemistry (9hrs)

Historical background. Classification and nomenclature. Alkyls and aryls of main group metals. Organometallic compounds of transition metals. The 18-electron rule- electron counting by neutral atom method and oxidation state method. The 16-electron rule. Metal carbonyls-Synthesis, structure, bonding and reactions. Nytrosyl, dihydrogen and dinitrogen complexes. Transition metal to carbon multiple bond-metal carbenes and carbines.

Unit 2: Organometallic Compounds of Linear and Cyclic π-Systems (9hrs)

Transition metal complexes with linear π- systems - Hapticity. Sythesis, structure, bonding and properties of complexes with ethylene, allyl, butadiene and acetylene. Complexes of cyclic π-systems - Synthesis, structure, bonding and properties of complexes with cyclobutadiene, $C_5H_5^-$ C_6H_6, $C_7H_7^+$ and $C_8H_8^{2-}$. Fullerene complexes. Fluxional organometallics.

Unit 3: Organometallic Reactions and Catalysis (9hrs)

Organometallic reactions- ligand dissociation and substitution- Oxidative addition and reductive elimination. Insertion reactions involving CO and alkenes. Carbonylation by Collman`s reagent.
Electrophilic and Nucleophilic attack on coordinated ligand.
Homogeneous and heterogeneous catalysts.
Homogeneous catalysis by organometallic compounds: Hydrogenation by Wilkinson`s catalyst, Hydroformylation, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis.
Heterogeneous catalysis by organometallic compounds: Ziegler-Natta polymerizations, Fischer-Tropsch process and water gas shift reaction.

Unit 4: Metal Clusters (9hrs)

Metal-Metal bond and metal clusters. Bonding in metal-metal single,double,triple and quadruple bonded non-carbonyl clusters. Carbonyl clusters-electron count and structure of clusters. Wade-Mingos-Lauher rules. Structure and isolobal analogies. Carbide clusters. Polyatomic Zintl anions and cations. Chevrel phases.

Unit 5: Bioinorganic Chemistry-I (9hrs)

Occurrence of inorganic elements in biological systems- bulk and trace metal ions. Emergence of bioinorganic chemistry. Coordination sites in biologically important ligands. Ion transport across membranes. Role of alkali metal ions in biological systems. The sodium/potassium pump.

Structural role of calcium. Storage and transport of metal ions- ferritin, transferrin and siderophores. Oxygen transport by heme proteins-hemoglobin and myoglobin-structure of the oxygen binding site-nature of heme-dioxygen binding-cooperativity. Hemerythrin and hemocyanin.

Unit 6: Bioinorganic Chemistry-II (9hrs)

Metallo enzymes and electron carrier metallo proteins. Iron enzymes: Cytochrome P-450, catalase and peroxidase. Copper enzymes: Oxidase, superoxide dismutase and tyrosinase. Lewis acid role of Zn(II) and Mn(II) containing enzymes. Carboxypeptidase. Vitamin B_{12} and Coenzymes. Chlorophil II- Photosystem I and II. Nitrogen fixation-Nitrogenases. Anticancer drugs.

References:

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements,* 2/e, Elsevier Butterworth-Heinemann, 2005.
2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi, *Inorganic Chemistry, principles of structure and reactivity,* Pearson Education, 2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry,* Pearson, 2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry,* Oxford University Press, 2002
5. William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press, 2005.
6. Keith F Purcell, John C Kotz, *Inorganic Chemistry*, Cengage Learning, 2010.
7. James E House, *Inorganic Chemistry,* Academic Press, 2008.
8. B.Douglas, D.McDaniel, J.Alexander, *Concepts and Models of Inorganic Chemistry,* Wiley Student Edition, 2006.
9. F.A.Cotton and G.Wilkinson, *Advanced Inorganic Chemistry,* Wiley.
10. R.C.Mehrothra and A.Singh, *Organometallic Chemistry, A Unified Approach, W*iley Eastern.
11. P.Powell, *Principles of Organometallic Chemistry, ELBS.*
12. B.D.Gupta and A.J.Elias, *Basic Organometallic Chemistry, Concepts, Synthesis and Applications,* Universities Press, 2010.
13. Piet W.N. M.van Leeuwen, *Homogeneous Catalysis*, Springer, 2010.
14. S.J. Lippard and J.M.Berg, *Principles of Bioinorganic Chemistry*, University Science Books.
15. I. Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, *Bioinorganic Chemistry, Viva Books Pvt. Ltd., 1998.*

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

CH3C11 - REAGENTS AND TRANSFORMATIONS IN ORGANIC CHEMISTRY (3Credts, 54hrs)

Unit 1: Oxidations (9hrs)

Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium). Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Prevost and Woodward dihydroxylations, Sharpless asymmetric dihydroxylation. Allylic oxidation with CrO_3^- Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O_3. Oxidative decarboxylation, Riley reaction, Baeyer -Villiger oxidation, Dess-Martin oxidation, Swern oxidation, hydroboration-oxidation.

Unit 2: Reductions (9hrs)

Catalytic hydrogenation of alkenes and other functional groups (heterogeneous and homogeneous), Noyori asymmetric hydrogenation, hydrogenolysis. Liquid ammonia reduction with alkali metals. Metal hydride reductions. Reduction of carbonyl group with hydrazine, p-tosylhydrazine, diimide and semicarbazide. Clemmensen reduction, Birch reduction. Wolff-Kishner reduction, Bouveault-Blanc reduction, MPV reduction, hydroboration, Pinacol coupling, McMurry coupling, Shapiroreaction.

Unit 3: Synthetic Reagents (9 hrs)

Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, LiAlH4, LiBH4, DIEA, BuLi, diborane, 9-BBN, t-butoxycarbonylchloride, DCC, Gilman's reagent, lithium dimethyl cuprate, tri-n-butyltinhydride, 1,3-dithiane, trimethyl silyl chloride, $Pb(OAc)_4$, ceric ammonium nitrate, DABCO, DMAP, DBU, DDQ, DEAD and Lindlar catalyst in organic synthesis.

Unit 4: Chemistry of Polymers (9 hrs)

Classification of polymers, chain, step, free-radical and ionic polymerizations. Plastics, rubbers and fibers, thermosets and thermoplastics, linear, branched, cross-linked and network polymers, block and graft copolymers.
Natural and synthetic rubbers.
Biopolymers: Primary, secondary and tertiary structure of proteins, Merrifield solid phase peptide synthesis, Protecting groups, sequence determination of peptides and proteins, Structure and synthesis of glutathione, structure of RNA and DNA, structure of cellulose and starch, conversion of cellulose to rayon.

Unit 5: Chemistry of Heterocyclic Compounds (9 hrs)

Aromatic and nonaromatic heterocyclics, structure, synthesis and reactions of a few heterocyclics- aziridine, oxirane, azetidine, pyrrole, furan, thiophene, indole, pyridine, quinoline, imidazole, oxazole, pyrazole, and thiazole. Synthesis of uracil, thymine, cytosine, adenine and guanine. Structure and synthesis of Uric acid and Caffeine.

Unit 6: Molecular Rearrangements and Transformations (9hrs)

Rearrangements occurring through carbocations, carbanions, carbenes and nitrenes such as Wagner-Meerwein, Demjanov, dienone-phenol, benzil- benzilic acid, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Fries, Bayer-Villiger, Wittig, Orton, and Fries rearrangements. Peterson reaction, Woodward and Prevost hydroxylation reactions. Heck, Negishi, Sonogashira, Stille, and Suzuki coupling reactions (mechanism only).

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
2. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis,* 3/e, CRC Press, 1998.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge University Press.
4. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer, 2007.
5. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
7. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.

8. V. K. Ahluwalia and R. Aggarwal, *Organic Synthesis: Special Techniques*, 2/e, Narosa Publishing House, 2006.
9. G. Odiyan, *Principles of Polymerisation*, 4/e, Wiley, 2004.
10. V.R. Gowriker and Others, *Polymer Science*, Wiley Eastern Ltd.
11. I.L. Finar, *Organic Chemistry*, Vol. II, 5/e, ELBS, 1975.
12. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press, 2004.
13. T. L. Gilchrist, *Heterocyclic Chemistry*, 3/e, Pearson, 1997.
14. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

CH3E01 - SYNTHETIC ORGANIC CHEMISTRY
(3 Credits, 54hrs)

Unit 1: Reagents for Oxidation and Reduction (9hrs)

Reagents for oxidation and reduction: Oxone, IBX, PCC, osmium tetroxide, ruthenium tetroxide, selenium dioxide, molecular oxygen (singlet and triplet), peracids, hydrogen peroxide, aluminum isopropoxide, periodic acid, lead tetraacetate. Wacker oxidation, TEMPO oxidation, Swern oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation. Catalytic hydrogenations (heterogeneous and homogeneous), metal hydrides, Birch reduction, hydrazine and diimide reduction.

Unit 2: Organometallic and Organo-nonmetallic Reagents (9hrs)

Synthetic applications of organometallic and organo- nonmetallic reagents: Reagents based on chromium, nickel, palladium, silicon, and born, Gilman reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes. Gilman's reagent, Tri -n-butyl tin hydride, Benzene Tricarbonyl Chromium

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylicacids, esters, acyl halides, amides. Substitution at α-carbon, aldol and related reactions, Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfur ylides. Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Introduction to combinatorial chemistry.

Unit 4. Coupling Reactions (9hrs)

Coupling Reactions: Palladium Catalysts for C-N and C-O bond formation, Palladium catalyzed amine arylation (Mechanism and Synthetic applications). Sonogashira cross coupling reaction (Mechanism, Synthetic applications in Cyclic peptides) Stille carbonylative cross coupling reaction (Mechanism and synthetic applications). Mechanism and synthetic applications of Negishi, Hiyama, Kumada, Heck and Suzuki-Miyaura coupling reactions.

Unit 5: Multi step Synthesis (9hrs)

Multi step Synthesis**:** Synthetic analysis and planning, Target selection, Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, uplong reactions and use in synthesis. Introduction to retrosynthetic analysis, Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone.

Unit 6: Retro Synthetic Analysis and Heterocyclics (9hrs)

Retrosynthesis: General principles of retrosynthetic analysis-synthons and reagents, donor and acceptor synthons, umpolung, protecting group chemistry and functional group interconversions. One group and two group C-X and C-C disconnections, functional group transposition. Examples for a few retrosynthetic analyses- paracetamol from phenol, benzocain from toluene and propranolol from 1-naphthol.

Structure, synthesis and reactions of fused ring heterocycles: Benzofuran, Indole, Benzothiophene, Quinoline, Benzoxazole, Benzthiazole, Benzimidazole, Triazoles , Oxadiazoles and Tetrazole. Structure and synthesis of Azepines, Oxepines, Thiepins, Diazepines and Benzodiazepines. Structure and synthesis (Reichstein process) of Vitamin C (Reichstein process).

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
2. S. Warren and P. Wyatt, *Organic Synthesis: Strategy and Control*, John Wiley
3. S. Warren: *Organic Synthesis: The Disconnection Approach*, John Wiley
4. H. O. House: *Modern Synthetic Reactions*, W. A. Benjamin
5. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge University Press.
6. T. W. Greene and P. G. M. Wuts: *Protecting Groups in Organic Synthesis*, 2nd ed., John Wiley
7. M B Smith and J. March: *Advanced Organic Chemistry-Reactions, Mechanisms and Structure*, 6th ed., John Wiley
8. T. H. Lowry and K. S. Richardson: *Mechanism and Theory in Organic Chemistry*, 3rd ed.
9. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part A and B, 5/e, Springer, 2007
10. A. Pross: *Theoretical and Physical Principles of Organic Chemistry*, John Wileyumada, Heck and Suzuki-Miyaura coupling reactions.
11. T.W. Graham Solomons: *Fundamentals of Organic Chemistry*, 5th ed., John Wiley
12. I. L. Finar: *Organic Chemistry* Volumes 1 (6th ed.), Pearson
13. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2/e, Oxford University Press
14. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
15. N. K. Terret: *Combinatorial Chemistry*, Oxford University Press, 1998

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

CH4C12 INSTRUMENTAL METHODS OF ANALYSIS
(4 Credits, 72 hrs)

Unit 1: **Errors in Chemical Analysis (9hrs)**

Treatment of analytical data, accuracy and precision, Absolute and relative errors, classification and minimization of errors, significant figures, Statistical treatment-mean and standard deviation, variance, confidence limits, student-t and f tests, detection of gross errors, rejection of a result-Q test. Least square method, linear regression; covariance and correlation coefficient.

Unit 2: **Conventional Analytical Procedures (9hrs)**

Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ and NH_4SCN.
Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-lnaphthol, dithiocarbamates, Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions.
Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations.
Redox titrations: Permanganometry, dichcrometry, iodometry, cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators.
Precipitation titrations, adsorption indicators.
Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

Unit 3: Electro Analytical Methods- I (9hrs)

Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Polarography micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.

Unit 4 Electro Analytical Methods II (9hrs)

Amperometry: biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

Unit 5 Optical Methods - I (9 hrs)

Fundamental laws of spectrophotometry, nephelometry and turbidometry and fluorimetry. UV-Visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations. Atomic emission spectrometry – excitation sources (flame, AC and DC arc), spark, inductively coupled plasma, glue discharge, laser microprobes, flame structure, instrumentation, and qualitative and quantitative analysis. Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications.

Unit 6 Optical Methods - II (9 hrs)

Theory, instrumentation and applications of: - Atomic fluorescence spectrometry, X-ray methods,: X-ray absorption and X-ray diffraction, photoelectron spectroscopy, Auger, ESCA. SEM, TEM, AFM.

Unit 7: **Thermal and Radiochemical Methods (9hrs)**

Thermogravimetry(TG), Differential Thermal Analysis(DTA) and Differential Scanning Calorimetry(DSC) and their instrumentation. Thermometric Titrations.

Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications.Principle and applications of isotope dilution methods.

Unit 8: Chromatography (9 hrs)

Chromatography-classification-column-paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel Permeation Chromatography.

Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC

References:

01. J.M. Mermet, M. Otto, R. Kellner, *Analytical Chemistry*, Wiley-VCH, 2004.

02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of Analytical Chemistry*, 9th Edn., Cengage Learning., 2014.
03. J.G. Dick, *Analytical Chemistry*, R.E. Krieger Pub.,1978.50
04. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Pub., 1990.
05. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative Chemical Analysis*, 5th Edn., John Wiley& sons,1989.
06. C.L. Wilson, D.W. Wilson, *Comprehensive Analytical Chemistry*, Elsevier, 1982.
08. G.D. Christian, J.E. O’Reilly, *Instrumental Analysis*, Allyn & Bacon, 1986.
09. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
10. A.I. Vogel, *A Textbook of Practical Organic Chemistry*, 5/e Pearson, 1989.
11. H.A. Laitinen, W.E. Harris, *Chemical Analysis*, McGraw Hill,1975.
12. V.K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, CRC, 2008.
13. F.W. Fifield, D. Kealey, *Principles and Practice of Analytical Chemistry*, Blackwell Science, 2000.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

CH4C13- ADVANCED TOPICS IN CHEMISTRY (4Credits, 72hrs)

Unit 1: Chemistry of Nanomaterials (9hrs)

History of nanomaterials- Classification.Size- dependence of properties. Electronic structure theory of metals and semiconductors. Quantum size effects.

Synthesis of nanostructures: bottom-up-approach, top- down approach, self-assembly, lithography, molecular synthesis, template assisted synthesis.

Methods of characterization: Electron microscopies-SEM,TEM. Scaning prob microscopies-STM, AFM. X-ray photoelectron spectroscopy(XPS), Dynamic light scattering(DLS), X-ray diffraction(XRD).

Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofilteration, diagnostic and therapeutic applications and targeted drug delivery. Introduction to graphenes and fullerenes.

Unit 2: Green Chemistry (9hrs)

Introduction, the need of green chemistry, principles of green chemistry, planning of green synthesis, tools of green chemistry. Green reactions- Aldol condensation, Cannizaro reaction and Grignard reaction.Comparison of the above green reactions with classical reactions.Green preparations. Applications of phase transfer catalysis. Introduction to microwave organic synthesis, Applications: environmental, solvents, time and energy benefits.

Unit 3: Introduction to Computational Quantum Chemistry (9hrs)

Electronic structure of molecules-Review of Hartee-Fock SCF method. Basis sets STOs and GTOs . Nomenclature of Basis sets. Semi empirical and ab initio methods. Calculations using Gaussian programme . Spesification of molecular geometry using a) Cartisian coordinates and b) Internal coordinates. The Z-matrix . Z- matrices of some simple molecules like H_2,H_2O, formaldehyde ammonia and methanol

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Unit 4: Supramolecular Chemistry (9hrs)

Concepts and language. Molecular recognition: Molecular receptors for different types of molecules, design and synthesis of coreceptors and multiple recognition. Strong, weak and very weak Hydrogen bonds.Utilisation of H-bonds to create supramolecular structures. Use of H bonds in crystal engineering and molecular recognition.

Supramolecular reactivity and catalysis. Transport processes and carrier design.

Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices Some examples of self- assembly in supramolecular chemistry.

Unit 5: Medicinal Chemistry (9hrs)

Drug Design and Relationship of Functional Groups to Pharmacologic Activity: Introduction, different classes of drugs, drug action, pro drugs, physico chemical properties of drugs and their pharmacologic activity , SAR and QSAR , factors governing ability of drugs. Drug design, factors governing drug design, rational approach to drug design, general methods of drug synthesis.

Immunoassays: General principles, antigen -antibody interactions, Hapten inhibition test, immunodiffusion, immunoelectrophoresis, ELISA, ELOSA, Fluorescence immunoassay and Radio immunoassay. Biosensors and chemosensors (basic idea only).

Unit 6: Combinatorial Chemistry (9hrs)

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, requirements-resins, Linkers. Reactants for solid phase synthesis. Methods of Parallel synthesis: Haughton`s tea bag procedure. Automated parallel synthesis. Methods in mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis. Structure determination of active compounds- Deconvolution. Methods in deconvolutionrecursive deconvolution, tagging use of decoded sheets. Planning and designing of combinatorial synthesis. Spider like scaffolds, drug molecules. Limitations of combinatorial chemistry.

Unit 7: Introduction to Industrial Catalysis (9hrs)

Structure and chemical nature of surfaces. Physisorption and chemisorptions. Energy exchange at surface. Determination of surface area and pore structure of catalysts - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorptions methods. Determination of surface acidity-TPD method. Catalyst selectivity, effect of pore size on selectivity. Homogeneous and heterogeneous catalysts. Preparative methods for heterogeneous catalysts-precipitation and coprecipitation methods, sol gel method, flame hydrolysis. Preparation of Zeolites and silica supports. Mesoporous materials. Introduction to Phase transfer catalysis, biocatalysis, nanocatalysis and polymer supported catalysis. Application of heterogeneous catalysts in water gas shift reaction, ammonia synthesis, catalytic cracking, Fisher-Tropsch process, threeway catalysis.

Unit 8: Renewable Energy Sources (9hrs)

World's reserve of commercial energy sources and their availability, various forms of energy, Renewable and conventional energy systems, comparison - coal, oil and natural gas, availability, applications, merits and demerits. Renewable energy sources - solar energy, nature of solar radiation, components- solar heaters, solar cookers, water desalination. Photovoltaic generation – basics, merits and demerits of solar energy. i) Solid state junction solar cells:- principle of solar cells, Fabrication of CdS/Cu_2S and $CdS/CuInSe_2$ solar cells, performance testing, stability and efficiency consideration. Dye sensitized solar cells (DSSC)-Working principle, Fabrication of DSSCs based on TiO2 and ZnO, stability and performance of dyes.

References:

1. C.P.Poole(Jr.) and F.J. Owens, *Introduction to Nanotechnology*,Wiley India, 2007.
2. G.A.Ozin and A.C.Arsenault, *Nanochemistry*, RSC Publishing,2008.
3. T.Pradeep, *The essentials of Nanotechnology*, Tata McGra Hill, New Delhi, 2007.
4. K.J.Klabunde(Ed.), *Nanoscale Materials in Chemistry*, John Wiley&Sons, 2001.
5. P.T.Anastas and J.C.Warner, *Green Chemistry:Theory and Practice,* Oxford University Press, 1998.
6. James Clark and Duncan Macquarrie, *Hand Book of Green Chemistry and Technology*, Blackwell Science, 2002.
7. J.H.Clark,*The Chemistry of waste minimization,* Blackie Academic, London,1995.
8. C.J.Cramer, *Essentials of computational Chemistry:Theories and models*, John Wiley & Sons,2002.
9. Frank Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons,1999.
10. Errol G Lewars *Computational Chemistry*: *Introduction to the theory and applications of molecular quantum mechanics*, Springer,2001.
11. David Young, *Computational Chemistry*, Wiley –Interscience, 2001.
12. F. Vogtle, *Supramolecular Chemistry,* John Wiley & Sons, Chichester, 1991.
13. J.M.Lehn, *Supramolecular Chemistry*, VCH.
14. Lemke, Williams, Roche and Zito, *Principles of Medicinal Chemistry*, 7/e, Wolters Kluwer, 2012.
15. G.Thomas, *Fundamentals of Medicinal Chemistry,* Wiley.
16. G.Gringauz, *Introduction to Medical Chemistry*, Wiley-VCH, 1997.
17. Harkishan Singh and V.K.Kapoor, *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan, 2008.
18. W.Bannwarth and B.Hinzen, *Combinatorial Chemistry-From Theory to Application, 2^{nd}* Edition, Wiley-VCH, 2006.
19. A.W.Czarnik and S.H.DeWitt, *A Practical Guide to Combinatorial Chemistry,* 1st Edition, American Chemical Society, 1997.
20. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6 Edn., Wiley, 2011.
21. Jens Hajen, *Industrial Catalysis: A Practical Approach.* 2nd Edn., Wiley VCH, 2006.
22. Dipak Kumar Chakrabarty, *Adsorption and Catalysis by Solids,* New Age. 2007.
23. C.H. Bartholomew and R.J. Farrauto, *Fundamentals of Industrial Catalysis Process,* 2nd Edn. Wiley & Sons Inc. 2006.
24. Woodruff, D. P. and Delchar T. A., *Modern Techniques of Surface Science*, Cambridge Solid State Science Series, 1994.
25. Kurt K. Kolasinski, *Surface Science: Foundations of Catalysis and Nanoscience,* 3rd Edn., Wiley U. K., 2012.
26. Bansal N K, Kleeman M and Mells M, *Renewable Energy Sources and Conversion Technology,* Tata McGraw-Hill. (1990)
27. Kothari D.P., *"Renewable energy resources and emerging technologies",* Prentice Hall of India Pvt. Ltd., 2008.
28. Rai G.D, *"Non-Conventional energy Sources",* Khanna Publishers, 2000.

29. Michael Grätzel, *J. Photochemistry and Photobiology C: Photochemistry Reviews* 4 (2003) 145–153, *Solar Energy Conversion by Dye-Sensitized Photovoltaic Cells*, Inorg. Chem., Vol. 44, No. 20, 2005 6841-6851.
30. Yoshihiro Hamakawa, Thin-Film Solar Cells-Next *Generation Photovoltaics and Its Applications*, Springer Series in Photonics 13, 2004.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

CH4EO5 - INDUSTRIAL CATALYSIS (ELECTIVE) (4 Credits, 72hrs)

Unit 1: Introduction to Adsorption process (9hrs)

Intermolecular interactions, physisorption – the forces of adsorption – dispersion and repulsive forces – classical electrostatic interactions – adsorbate-adsorbate interactions, chemisorption, potential energy curves, thermodynamics of adsorption – isothermal and adiabatic heats of adsorption – variation of heats of adsorption with coverage, adsorption isotherms, Langmuir, BET and Freundlich, kinetics of chemisorption – activated and non-activated chemisorption – absolute rate theory – electronic theories, hysteresis and shapes of capillaries.

Unit 2: Kinetics and Catalysis (9hrs)

Adsorption and catalysis – adsorption and reaction rate – strength of adsorption bond and catalysis – adsorption equilibrium and catalysis, kinetics of heterogeneous catalysis: diffusion steps neglected – unimolecular reactions – bimolecular reactions – Langmuir-Hinshelwood and Eley-Rideal mechanism, kinetics of heterogeneous catalysis: diffusion controlling – mechanism of diffusion – diffusion and reaction in pores – selectivity and diffusion, electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.

References:

1. A. Clark, *"Theory of adsorption and catalysis",* Academic Press, 1970.
2. J.M. Thomas & W.J. Thomas, *"Introduction to principles of heterogeneous catalysis",* Academic Press, New York, 1967.
3. R.H.P. Gasser, *"An introduction to chemisorption and catalysis by metals",* Oxford, 1985.
4. D.K Chakraborthy, *"Adsorption and catalysis by solids",* Wiley Eastern Ltd. 1990.

Unit 3: Catalyst - Praparative Methods(9hrs)

Surface area and porosity measurement – measurement of acidity of surfaces; Support materials– preparation and structure of supports – surface properties, preparation of catalysts – introduction of precursor compound – pre-activation treatment – activation process. General methods of synthesis of zeolites, mechanism of nuclear formation and crystal growth, structures of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Unit 4: Deactivation of Catalysts (9hrs)

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

References:

1. J.R. Anderson and M. Boudart (Eds), *"Catalysis, Science and Technology",* Vol 6, Springer-Verlag, Berlin Heildberg, 1984.
2. R.B. Anderson, *"Experimental methods in catalysis research",* Vol I, II, Academic press, NY, 1981.
3. R. Szostak, *"Molecular sieves: principles of synthesis and identification*", Van Nostrand, NY, 1989.
4. R. Hughes*, "Deactivation of catalysts",* Academic press, London, 1984.

UNIT 5: Phase Transfer Catalysis (9hrs)

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts. Use of quaternary salts – macrocyclic and macrobicyclic ligands – PEG's and related compounds –use of dual phase transfer catalyst or co-catalyst in phase transfer systems –separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

UNIT 6: Biocatalysis (9hrs)
Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes.

References:

1. C.M. Starks, C.L. Liotta And M. Halpern, *"Phase Transfer Catalysis – Fundamentals, Applications And Industrial Perspectives"*, Chapman & Hall, New York, 1994.
2. A.L. Lehninger, *"Principles of Biochemistry",* Worth Publishers, USA, 1987.

UNIT 7: Industrial Catalysis-1 (9hrs)

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

UNIT 8: Industrial Catalysis-II (9hrs)

Hydroformylation of olefins, carbonylation of organic substrates, conversion of methanol to acetic acid, synthesis of vinyl acetate and acetic anhydride, palladium catalyzed oxidation of ethylene, acrylonitrile synthesis, Zeigler-Natta catalysts for olefin polymerization. Propene polymerization with silica supported metallocene/MAO catalysts.

References:

1. G. Ertl, H. Knozinger and J. Weitkamp, *"Handbook of Heterogeneous Catalysis*" Vol 1-5, Wiley-VCH, Weinheim, 1997.

2. R.J. Farrauto and C.H. Bartholomew, *"Fundamentals of Industrial Catalytic Processes",* Blackie Academic and Professional – Chapman and Hall, 1997.

3. R. Pearce and W.R. Patterson, *"Catalysis and chemical processes*", Academic press, Leonard Hill, London, 1981.

M.Sc. CHEMISTRY – SEMESTER III & IV

CH3PO7 & CH4P10 – INORGANIC CHEMISTRY PRACTICALS– III & IV (4 Credits)

Unit 1: Estimation of ions in mixture

Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+}, $Nl^{2+,}$ Zn^{2+}, Fe^{3+}, Ca^{2+}, Mg^{2+}, Ba^{2+} and Cr_2O1^{2-}) by volumetric colorimetric or gravimetric methods only one of the components to be estimated.

Unit 2: Colorimetric Estimations

Colorimetric estimations of Ni, Cu, Fe and Mo, after separation from other ions in solution by solvent extraction. (Minimum two expts.)

Unit 3: Ion Exchange Methods

Ion- exchange separation and estimation of binary mixtures (Co^{2+} & $Ni^{2+,}$ Zn^{2+} & $Mg^{2+.}$ Hardness of water).

Unit 4: Preparation of Inorganic Complexes. (5 Nos)

References:

1. *Vogel's Text Book of Qualitative Inorganic Analysis*.
2. I.M. Kolthoff and E.A. Sanderson, *Quantitative Chemical Analysis.*
3. D.A. Adams and J.B. Rayner, *Advanced Practical Inorganic Chemistry*.
4. W.G.Palmer, *Experimental Inorganic Chemistry.*
5. G. Brauer, *Hand book of Preparative Inorganic Chemistry*.

M.Sc. CHEMISTRY – SEMESTER III & IV

CH3PO8 & CH4P11 – ORGANIC CHEMISTRY PRACTICALS– III & IV (4 Credits)

Unit 1: Quantitative Organic Analysis
Estimation of equivalent weight of acids by Silver Salt method, Estimation of nitrogen by Kjeldahl method, Determination of Acid value, iodine value and saponification value of oils and fats (at least one each), Estimation of reducing sugars, Estimation of amino group, phenolic group and esters. Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulpha drug (Sulpha diazine, sulphaguanidine), Antibiotics – Pencillin, Stroptomycin.

References:
1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, ELBS/Longman, 1989.
2. Beebet, *Pharmacuetical Analysis*.

Unit 2: Extractions
Extraction of Natural products and purification by column chromatography and TLC – Caffeine from Tea waste, Chlorophill Steroids, Flavonoid (Soxhlet extraction), citral from lemon grass (steam distillation). Casein from milk.

Unit 3: Chromatograhy
Practical application of PC and TLC, Preparation of TLC plates, Activation, Identification of the following classes of compounds using one- and two-dimensional techniques. Identification by using spray reagents and co-chromatography by authentic samples and also from Rf values. Food additives and Dyes, Artificial sweeteners: Saccharine, cyclamates, Dulcin. Flavour adulterants – piperonal, Benzalacetate, ethyl acetate antioxidants: Butylated hydroxytoluene (BHT) Butylated hydroxy anisole (BHA), Hydroquinone.

Food colours: Permitted – Amaranth, Erythrosine, Tatrazine, susnet yellow, Fast green, Brilliant Blue, Nonpermitted colours: Auramine, Congo red, Malachite green, Metanil yellow, Orange II, Sudan II, Congo red.
Amino acids (Protein hydrolysates), Sugars, Terpinoids, Alkaloids, Flavonoids, Steroids.
Pesticides and herbicides: Oragonochlorine pesticides organo phosphates and carbamate pesticides, Herbicides.
Plant growth stimulants: Indole acetic acid.

References:
1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5/e, Pearson, 1989.
2. Beebet, *Pharmacuetical Analysis*
3. E. Hoftmann, *Chromatography*, non Nostrand Reinhold Company, New York, 1975.
4. J. Sherma and G. Zwig, *TLC and LC analysis of pesticides of international importance*, Vol.

VI & VII, Academic Press.
5. H. Wagner, S. Bladt, E.M. Zgainsti – Tram, Th. A. Scott., *Plant Drug Analysis*, Springer-Verlag, Tokyo, 1984.
6. Vishnoi, *Practical Organic Chemistry*.

M.Sc. CHEMISTRY – SEMESTER III & IV

CH3PO9 & CH4P12 – PHYSICAL CHEMISTRY PRACTICALS– III & IV (4 Credits)

SECTION A

Unit 1: Chemical Kinetics (4 experiments)
1. Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids.
2. Determination of Arrhenius parameters of acid hydrolysis of an
3. Determination of specific reaction rate of saponification of ethyl
4. Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.

Unit 2: Adsorption (3 experiments)
1. Verification of Langmuir adsorption isotherm – charcoal-acetic acid system. Determination of the concentration of a given acetic acid solution using the isotherm
2. Verification of Langmuir adsorption isothem – charcoal-oxalic acid system. Determination of the concentration of a given acetic acid solution using the isothem.
3. Determination of surface area of adsorbent.

Unit 3: Phase Equilibria (2 experiments)
1. (a) Determination of phase diagram of a ternary liquid system (e .g.,chloroform – acetic acid – water – Benzene – acetic acid – water)
(b) Determination of the composition of a binary liquid mixture (e.g., chloroform-acetic acid, benzene-acetic acid)
2. (a) Determination of mutual miscibility curve of a binary li quid system (e.g., phenol – water) and critical solution temperature (CST).
(b) Effect of impurities (e.g, NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system
(c) Effect of a given impurity (e.g., KCl) on the CST of water –phenol system and determination of the concentration of the given solution of

Unit 4: Cryoscopy – Beckman Thermometer Method (3 experiments)
1. Determination of cyroscopic constant of a liquid (water, benzene)
2. Determination of molecular mass of a soute (urea, glucose, cane sugar,mannitol) by studying the depression in freezing point of a liquid solvent (water, benzene)
3. Determination of Van't Hoff factor and percentage of dissociation of NaCl.
4. Study of the reaction 2Kl $^{+}$ HgI 2 .K_2HgI_4 and determination of the concentration of the given KI solution.

Unit 5: Polarimetry (3 experiments)
1. Determination of specific and molar optical rotations of glucose, fructose and sucrose.
2. Determination of specific rate of inversion of cane sugar in presence of HCl.
3. Determination of concentration of HCl

Unit 6: Spectrophotometry (3 experiments)

1. Determination of equilibrium constants of acid -base indicators.
2. Simultaneous of determination Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$
3. Investigation of complex formation between Fe (III) and thiocyanate.

References:

1. A. Finlay and J.A. Kitchener, *Practical Physical Chemistry*, Longman.
2. F. Daniels and J.H. Mathews, *Experimental Physical Chemistry*, Longman.
3. A.H. James, *Practical Physical Chemistry* , J.A. Churchil Ltd., 1961.
4. H.H. Willard, L.L. Merit and J.A. Dean, *Instrumental Methods of Analysis*, 4th Education, Affiliated East-West Press Pvt. Ltd., 1965.
5. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry*, McGraw Hill.
6. J.B. Yadav, *Advanced Practical Physical Chemistry*, *Goel Publications*, 1989.

SECTION B

Use of Computational Chemistry softwares like pc GAMESS (firefly), Gaussian etc., to calculate molecular parameters.

Ref: http://classic.chem.msu.su/gran/gamess/index.html