Maharaja's College Ernakulam

A GOVERNMENT AUTONOMOUS COLLEGE

Re-Accredited by NAAC with 'A Grade'
Affiliated to Mahatma Gandhi University
Centre of Excellence under Govt. of Kerala
Identified by UGC as College with Potential for Excellence

POST GRADUATE & RESEARCH DEPARTMENT OF CHEMISTRY

Post Graduate Curriculum and Syllabus

(All Branches)

For 2019 Admission Onwards

M.Sc. CHEMISTRY

FOREWORD

The Board of Studies in Chemistry take this opportunity to express our deep appreciation to all academicians and professionals who participated in the series of workshops organized by the Board for restructuring curriculum and syllabi of the PG courses in Chemistry - M.Sc Chemistry, M.Sc Analytical Chemistry, M.Sc Pharmaceutical Chemistry and M.Sc Applied Chemistry. We express our profound gratitude to the Honourable Vice-Chancellor, Pro-Vice Chancellor, Members of the Syndicate and Members of the Academic Council, Mahatma Gandhi University, for their sincere co-operation and guidance for completion of this work. Our special thanks are due to Chairman and members of the Governing Council, Chairman and members of the Academic Council, Maharaja's College, Ernakulam.

We also extend our gratitude to Prof. (Dr). K. K. Mohammed Yusuff, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). S. Sugunan, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Girish Kumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Sreekumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Dr. E. Prasad, Associate Professor, Department of Chemistry, IIT, Madras, Dr. Kochubaby Manjooran, Dy.Manager (Energy and Envt), BPCL, Kochi Refinery, Sri. M. G. Rajagopalan, Associate Professor (Retd.) Maharaja's College, Ernakulam, Smt. K. T. Geethabali, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. T. Narayanan, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. Lissamma Koshy, Associate Professor (Retd.), Maharaja's College, Ernakulam and Dr. Anitha I, Principal, KKTM College, Pullut who were entrusted with the responsibility as experts for the revision of the syllabus of different subjects. The Board of Studies in Chemistry expresses the whole hearted gratitude to all those who have helped in this endeavour.

The task of preparing the curricula and syllabi and bringing it out in the present form for all the four M.Sc courses was not simple but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS and the faculty members of the Department of Chemistry. I would like to express my sincere thanks to all my fellow members of BOS and the faculty members of the Department of Chemistry for all their help, cooperation, encouragement, active participation and useful suggestions for the completion of syllabus.

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PROGRAMME STRUCTURE

Examination

- There shall be end semester examination at the end of each semester.
- The answers must be written in English except for those coming under Faculty of Languages.
- Practical examinations shall be conducted by the college at the end of even semesters only.
- Project evaluation and Viva -Voce shall be conducted at the end of the programme only.
- Practical examination, Project evaluation and Viva-Voce shall be conducted by two external examiners.

END-Semester Examination

- The examinations shall normally at the end of each semester. There shall be one end-semester examination of 3 hours duration in each lecture based course and practical course.
- A question paper may contain short answer type/annotation, short essay type questions/problems and long essay type questions.

Evaluation and Grading

Evaluation

The evaluation scheme for each course shall contain two parts; (a) in-semester evaluation and (b) end-semester evaluation. 20 marks shall be given to in-semester evaluation and the remaining 80 marks to end-semester evaluation. Both in-semester and end semester evaluation shall be carried out by using in mark system. Both internal and external marks are to be mathematically rounded to the nearest integer.

Internal evaluation

The internal evaluation shall be based on predetermined transparent system involving periodic written tests, assignments, seminars and attendance in respect of theory courses and based on written tests, lab skill/records/viva and attendance in respect of practical courses. The marks assigned to various components for in-semester evaluation is as follows.

Components of In-semester Evaluation (For theory)

Components	Component Marks
Assignment	4
Seminar	4
Two Test papers*	8
Attendance	4
Total	20

*Marks of Test Papers shall be the average

Components of In-semester Evaluation (For Practical)

Components	Component Marks
Attendance	4
Laboratory Involvement	4
Written/Lab Test	4
Record*	4
Viva	4
Total	20

*Marks awarded to Record should be related to number of experiments recorded

Components of In-semester Evaluation (For Project)

Components	Marks
Topic/Area selected	2
Experimentation/Data collection	4
Punctuality	2
Compilation	4
Content	4
Presentation	4
Total	**20**

a) Evaluation of Attendance

% of attendance	Mark
95 and above	4
85 to 94	3
80 to 84	2
75 to 79	1
< 75	0

(Decimals are to be rounded to the next higher whole number)

a) Evaluation of Assignment

Components	Marks
Punctuality	1
Content	1
Conclusion	1
Reference/Review	1
Total	**4**

b) Evaluation of Seminar

Components	Marks
Content	1
Presentation	2
Reference/Review	1
Total	**4**

To ensure transparency of the evaluation process, the in-semester marks awarded to the students in each course in a semester shall be published on the notice board at least one week before the commencement of external examination. There shall not be any chance for improvement for in semester marks. The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course and a copy should be kept in the college for at least one year for verification.

End-Semester Evaluation:

The end-semester evaluation in theory courses is to be conducted by the college with question papers set by external experts. The answers must be written in English except those for the Faculty of Languages. The evaluation of the answer scripts shall be done by examiners based on a well-defined scheme of valuation. The end-semester evaluation shall be done immediately after the examination preferably through Centralized Valuation.

Photocopies of the answer scripts of the external examination shall be made available to the students for scrutiny on request and revaluation/scrutiny of answer scripts shall be done as per the request of the candidate by paying fees.

The question paper should be strictly on the basis of model question paper set by BOS and there shall be a combined meeting of the question paper setters for scrutiny and finalization of question paper. Each set of question should be accompanied by its answer scheme for valuation.

Pattern of Questions

The question setter shall ensure that questions to course should satisfy weightage to objectives and weightage to difficulty levels.

Weightage to Objectives	
Objectives	**%**
Understanding	25
Critical Evaluation	50
Application	25

Weightage to difficulty levels	
Level of difficulty	**%**
Easy	20
Average	60
Difficult	20

Question paper setters shall also submit a detailed scheme of evaluation along with the question paper. A question paper shall be a judicious mix of objective type, short answer type, short essay type /problem solving type and long essay type questions.

Pattern of questions for end semester examination

	Total no. of questions	**Number of questions to be answered**	**Marks of each question**	**Total marks**
	12	10	2	20
	10	6	5	30
	4	2	15	30
TOTAL	**26**	**18**	x	**80**

Grades for Courses

For all courses (theory & practical), grades are given on a 10-point scale based on the total percentage of marks ***(ISA+ESA)*** as given below

Percentage of Marks	Grade	Grade Point (GP)
95 and above	S Outstanding	10
85 to below 95	A^+ Excellent	9
75 to below 85	A Very Good	8
65 to below 75	A- Good	7
55 to below 65	B^+ Above Average	6
50 to below 55	B Average	5
40 to below 50	C Pass	4
Below 40	F Fail	0
	Ab Absent	0

Credit Point and Credit Point Average:

Credit Point (CP) of a course is calculated using the formula

CP = C × GP, where C = Credit; GP = Grade point

Semester Grade Point Average (SGPA) of a Semester is calculated using the formula

SGPA= TCP/TC, where TCP = Total Credit Point of that Semester TC =

Total Credit of that Semester

Cumulative Grade Point Average (CGPA) of a Programme is calculated using the formula

CGPA = ∑(TCP ×TC)÷∑TC

CGPA shall be rounded off to two decimal places.

Grades for the different semesters and overall programme are given based on the corresponding CPA as shown below:

GPA	Grade
Equal to 9.5 and above	***S Outstanding***
Equal to 8.5 and below 9.5	***A+ Excellent***
Equal to 7.5 and below 8.5	***A Very Good***
Equal to 6.5 and below 7.5	***A- Good***
Equal to 5.5 and below 6.5	***B+ Above Average***
Equal to 5.0 and below 5.5	***B Average***
Equal to 4.0 and below 5.0	***C Pass***
Below 4.0	***F Failure***

M.Sc. CHEMISTRY

	Code	Course	Hours/ week	Total Hours	Credit	Marks		
						Internal	External	Total
Semester 1	PG1CHE C01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	4	72	4	20	80	100
	PG1CHE C02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	4	72	4	20	80	100
	PG1CHE C03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	4	72	4	20	80	100
	PG1CHE C04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	3	54	3	20	80	100
	PG2CHE P01	Inorganic Chemistry Practical–1	3	54	Evaluation at the end of second semester			
	PG2CHE P02	Organic Chemistry Practical-1	3	54				
	PG2CHE P03	Physical Chemistry Practical -1	4	72				
		Total	**25**	**450**	**15**			
Semester 2	PG2CHE C05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	4	72	4	20	80	100
	PG2CHE C06	Organic Chemistry- II (Reaction Mechanism)	4	72	4	20	80	100
	PG2CHE C07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	4	72	4	20	80	100
	PG2CHE C08	Physical chemistry- II (Molecular Spectroscopy)	3	54	3	20	80	100
	PG2CHE P01	Inorganic Chemistry Practical–1	3	54	3	20	80	100
	PG2CHE P02	Organic Chemistry Practical-1	3	54	3	20	80	100
	PG2CHE P03	Physical Chemistry Practical -1	4	72	3	20	80	100
		Total	**25**	**450**	**24**			
Semest	PG3CHE C09	Inorganic chemistry-III (Solid State Chemistry)	4	72	4	20	80	100

	PG3CHE C10	Organic chemistry- III (Organic Syntheses)	4	72	4	20	80	100
	PG3CHE C11	Physical chemistry- III (Chemical Kinetics, Surface Chemistry and Photochemistry)	4	72	4	20	80	100
	PG3CHE C12	Spectroscopic Methods in Chemistry	3	54	3	20	80	100
	PG4CHE P04	Inorganic Chemistry Practical–2	3	54	Evaluation at the end of fourth semester			
	PG4CHE P05	Organic Chemistry Practical-2	3	54				
	PG4CHE P06	Physical Chemistry Practical -2	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4CHE E01	Elective –I Inorganic Chemistry - IV (Advanced Inorganic Chemistry)	5	90	4	20	80	100
	PG4CHE E02	Elective –II Organic Chemistry-IV (Advanced Organic Chemistry)	5	90	4	20	80	100
	PG4CHE E03	Elective –III Physical Chemistry- IV (Advanced Physical Chemistry)	5	90	4	20	80	100
	PG4CHE E04	Elective –IV Polymer Chemistry	5	90	4	20	80	100
	PG4CHE E05	Elective –V Analytical Chemistry	5	90	4	20	80	100
	PG4CHE P04	Inorganic Chemistry Practical–2	3	54	3	20	80	100
	PG4CHE P05	Organic Chemistry Practical-2	3	54	3	20	80	100
	PG4CHE P06	Physical Chemistry Practical -2	4	72	3	20	80	100
	PG4CHE D01	Project			2		100	100
	PG4CHE V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1CHE C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory- M.O energy level diagrams for octahedral and tetrahedral complexes with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

2.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

2.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

2.3 Electron transfer reactions: outer sphere mechanism- Marcus theory, inner sphere mechanism-Taube mechanism.

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

3.1 Organometallic compounds with linear π- donor ligands- olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

3.2 Complexes with cyclic π-donors- metallocenes and cyclic arene complexes structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

3.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters- LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade Mingos rules, cluster valence electrons.

Module 4: Electron deficient compounds (9 Hrs)

4.1. Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds. Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines – Structure and bonding of borazines and Borides.

Module 5: Nuclear Chemistry (9 Hrs)

5.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

5.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology.

References

[1] J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4^{th} Edn., Harper Collins College Publishers,1993.

[2] F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6^{th} Edn., Wiley-Interscience, 1999.

[3] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

[4] P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall,1988.

[5] F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.

[6] B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

[7] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

[8] H.J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.

[9] S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

PG1CHE C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.

1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems, azulenes, annulenes, mesoionic compounds. NMR as a tool for aromaticity. Antiaromatic and homoaromatic systems. Fullerenes, Carbon nanotubes and Graphene.

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanohydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

4.1 Stereoisomerism: Definition based on symmetry and energy criteria. Projection formulae. Configurational isomerism. Geometrical isomerism- nomenclature, methods of determination of geometrical isomers based on physical properties, NMR spectroscopy and chemical methods. Optical isomerism, nomenclature.

4.2 Introduction to molecular symmetry and chirality: Examples from common objects to molecules. Axis, plane, center and alternating axis of symmetry.

4.3 Center of chirality: Molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

4.5 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

4.6 Chiral drugs.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Bridged bicyclic systems- norbornane, camphor, bicyclo[2.2.2]octane.

5.2. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle.

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

[2] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976. [3

[3] I. Fleming, Molecular Orbitals and Organic Chemical Reactions, Wiley, 2009.

[4] H.O. House, Modern Synthetic Reactions, Organic Chemistry Monograph Series, Benjamin, 1965.

[5] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

[6] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th Edn., Springer Science & Business Media, 2007.

[7] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[8] M.B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edn., John Wiley & Sons, 2007.

[9] M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edn., John Wiley & Sons, 2013.

[10] T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd Edn., Harper & Row, 1981.

[11] P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th Edn., Pearson

Education India, 1986.

[12] N.S. Isaacs, Physical Organic Chemistry, ELBS/Longman, 1987.

[13] D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3rd Edn., New Age Pub. Ltd., 2010.

[14] D.G. Morris, Stereochemistry, RSC, 2001.

[15] E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 2008.

[16] P.S. Kalsi, Stereochemistry, Conformation and Mechanism, 5th Edn., New Age International Pub. Ltd., 2004.

PG1CHE C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Formulation of Quantum Chemistry **(18 Hrs)**

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box-separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry **(18 Hrs)**

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

One-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

Rotational motion: co-ordinate systems, Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. The wave equation in Spherical polar coordinates-particle on a ring, the Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

3.2 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O as example).

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory (18 Hrs)

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

4.3 Applications in vibrational spectra: symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Determination of the symmetry of normal modes of H_2O, Trans-N_2F_2 and NH_3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra- determination of the number of active IR and Raman lines.

4.4 Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

References

[1] I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.

[2] P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.

[3] D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

[4] J.P. Lowe, K. Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006.

[5] R. Anatharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2001.

[6] R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

[7] T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006.

[8] H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006.

[9] L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.

[10] M.S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984.

[11] F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.

[12] L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969.

[13] V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

[14] S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

[15] S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn., Wiley, 2007.

[16] A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2000.

[17] A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010.

PG1CHE C04 - PHYSICAL CHEMISTRY - I

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Kinetic theory **(9 Hrs)**

Kinetic theory of gases, derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics **(18 Hrs)**

2.1 Entropy, dependence of entropy on variables of a system (S, T and V; S, T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

2.2 Free energy, Maxwell relations and significance, temperature dependence of free energy, Gibbs-Helmholtz equation, applications of Gibbs-Helmholtz equation.

2.3 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

2.4 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

2.5 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions- free energy, enthalpy, entropy andvolume. Determination of excess enthalpy and volume.

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

2.7 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

2.8 Three component systems- graphical representation. solid-liquid equilibria- ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria- one pair of partially miscible liquids, two pairs of partially miscible liquids, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

3.1 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations, the principle of microscopic reversibility, the Onsager reciprocal relations thermal osmosis, thermoelectric phenomena.

3. 2 Bioenergetics: Coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Module 4: Statistical Thermodynamics (18 Hrs)

4.1 Permutation, probability, apriori and thermodynamic probability, Stirling's approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function- translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

4.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

References

[1] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[2] K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.

[3] G.W. Castellan, Physical Chemistry, Addison-Wesley, 1983.

[4] R.P. Rastogi, R.R. Misra, An introduction to Chemical Thermodynamics, Vikas Publishing House, 1996.

[5] J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.

[6] M.C. Gupta, Statistical Thermodynamics, New Age International, 2007.

[7] M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981.

[8] I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglis, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall, 2002.

[9] L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn., Addison-Wesley, 1972.

[10] D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.

[11] F.W. Sears and G.L. Salinger, An Introduction to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addison-Wesley.

[12] C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.

[13] R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill, 1999.

SEMESTER 2

PG2CHE C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

Credits: 4 **Contact Lecture Hours: 72**

Module 1: Bioinorganic Compounds **(18 Hrs)**

1.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis- chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

1.2 Oxygen carriers and oxygen transport proteins- haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems- ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes- Carboxypeptidase A- structure and functions. Nitrogen fixation- nitrogenase, vitamin B_{12} and vitamin B_{12} coenzymes.

1.3 Metals in medicine- therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals (Cd, Hg, Cr and Pb).

Module 2: Inorganic Chains **(9 Hrs)**

2.1 Chains - catenation, homo and heterocatenation. Silicate minerals. Structure of silicates common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Silicones. Zeolites synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Phosphate esters in biological systems. Polythiazil- one dimensional conductors.

Module 3: Spectral and Magnetic Properties of Metal Complexes **(18 Hrs)**

3.1 Electronic Spectra of complexes- Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition- effect of spin orbit coupling and vibronic coupling.

3.2 Interpretation of electronic spectra of complexes- Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

3.3 Magnetic properties of complexes- paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism- inter and intra molecular interaction. Anomalous magnetic moments.

3.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Module 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds.

4.2 Linkage isomerism- electronic and steric factors affecting linkage isomerism. Symbiosis- hard and soft ligands, Prussian blue and related structures, Macrocycles- crown ethers.

Module 5: Reactions of Organometallic Compounds (9 Hrs)

5.1 Substitution reactions- nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

5.2 Addition and elimination reactions- 1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

5.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Module 6: Catalysis of Organometallic Compounds (9 Hrs)

6.1 Alkene hydrogenation, Tolman catalytic loop, Synthesis gas, Hydroformylation, Monsanto Acetic acid process, Wacker process, Zeigler Natta catalysis.

References

[1] F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3^{rd} Edn., Interscience,1972.

[2] J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4^{th} Edn., Pearson Education India, 2006.

[3] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

[4] R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984.

[5] B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3^{rd} Edn., Wiley-India, 2007.

[6] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

[7] R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

[8] B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.

[9] J.D. Lee, Concise Inorganic Chemistry, 4^{th} Edn., Wiley-India, 2008, 17.

[10] A.B.P. Lever, Inorganic Electronic Spectroscopy, 2^{nd} Edn., Elsevier, 1984.

PG2CHE C06 ORGANIC CHEMISTRY - II

(REACTION MECHANISM)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Chemistry of Carbocations **(9 Hrs)**

1.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

1.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Prins reaction, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions **(18 Hrs)**

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions- mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

2.5 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes **(9 Hrs)**

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

3.3 Arynes: generation, structure, stability and reactions. Orientation effect, amination of haloarenes.

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection of radical intermediates and its (a) addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements. Hydroperoxide: formation, rearrangement and reactions. Autoxidation.

4.2 Name reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry (9 Hrs)

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions**.**

References

[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

[2] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

[3] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edn., Springer Science & Business Media, 2007.

[4] W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.

[5] J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., Wiley, 2007.

[6] T.H. Lowry, K.H. Richardson, Mechanism and Theory in Organic Chemistry, Harper & Row, Publishers, Inc., New York, 1976.

[7] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

[8] S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.

[9] R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry, 7th Edn., Pearson, 2011.

[10] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[11] N.J. Turro, V. Ramamurthy, J.C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science books, 2009.

[12] N.J. Turro, Modern Molecular Photochemistry, Benjamin Cummings, 1978.

[13] K.K.R. Mukherjee, Fundamentals of Photochemistry, New Age Pub. Ltd, 1978.

[14] Jagadamba Singh, Jaya Singh, Photochemistry and Pericyclic Reactions, 3rd Edn., New Age International Publ. Ltd.

PG2CHE C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Approximate Methods in Quantum Mechanics (18 Hrs)

1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D – box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms- symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Module 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond order and free valency.

Module 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, and PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{3v}, C_{2h}, C_3 and D_{3h} groups. MO diagram for water and ammonia.

Module 4: Computational Chemistry (18 Hrs)

4.1 Introduction: computational chemistry as a tool and its scope.

4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.

4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments of quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.4 Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Interaction (CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.

4.6 General introduction to semiempirical methods: basic principles and terminology.

4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.8 Model Chemistry-notation, effect on calculation time (cost).

4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input- Cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

5.2 Identifying a successful GAMESS/Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.

5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

References

[1] I.N. Levine, Quantum Chemistry, 6^{th} Edn., Pearson Education, 2009.

[2] D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

[3] R.K. Prasad, Quantum Chemistry, 3^{rd} Edn., New Age International, 2006.

[4] F.A. Cotton, Chemical Applications of Group Theory, 3^{rd} Edn., Wiley Eastern,1990.

[5] V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

[6] A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010.

[7] E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2^{nd} Edn., Springer, 2011.

[8] J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

[9] F. Jensen, Introduction to computational chemistry, 2^{nd} Edn., John Wiley & Sons, 2007.

[10] A. Leach, Molecular Modeling: Principles and Applications, 2^{nd} Edn., Longman, 2001.

[11] J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.

[12] K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.

[13] A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons,2008.

[14] C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.

[15] D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

01. **Firefly / PC GAMESS** available from http://classic.chem.msu.su/gran/gamess/
02. **WINGAMESS** available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2CHE C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width-contributing factors, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non-radiative processes), relaxation time.

1.2 Microwave spectroscopy: principal moments of inertia and classification of molecules (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max}, effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

2.2 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

2.3 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

Module 3: Resonance Spectroscopy **(18 Hrs)**

3.1 NMR spectroscopy : Interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

3.2 FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

3.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

3.4 An elementary study of NQR spectroscopy.

References

[1] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

[2] G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.

[3] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[4] R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.

[5] R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

[6] K.J. Laidler, J.H. Meiser, Physical Chemistry, 2^{nd} Edn., CBS, 1999.

[7] W. Kemp, NMR in chemistry-A Multinuclear Introduction, McMillan, 1986.

[8] H. Kaur, Spectroscopy, 6^{th} Edn., Pragati Prakashan, 2011.

[9] H. Gunther, NMR Spectroscopy, Wiley, 1995.

[10] D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.

[11] D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.

[12] D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007.

[13] D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, EQR, I.K. International Publishing House Pvt. Limited, 2009.

SEMESTERS 1 AND 2

PG2CHE P01 INORGANIC CHEMISTRY PRACTICAL – 1

Credit: 3 **Contact Lab Hours: 54 + 54 = 108**

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - Ag^+, Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, Sn^{2+}, Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^+, Na^+, K^+, NH_4^+ (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

Colorimetric estimation of Cr, Fe, Ni, Mn, Cu, NH_4^+, nitrate and phosphate ions.

PART IV

Preparation and characterization of complexes using IR, NMR and electronic spectra.

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.

[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.

[3] V.V. Ramanujam, Inorganic Semi micro Qualitative Analysis, The National Publishing Co., Chennai.

[4] I. M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn, McMillian, 1968.

PG2CHE P02 ORGANIC CHEMISTRY PRACTICAL - 1

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture of two components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

1. Cycloaddition of diene and dienophile (Diels-Alder reaction).
2. Oxidation of primary alcohol to aldehyde and then to acid.
3. Benzoin condensation.
4. Esterification of simple carboxylic acids.
5. Aldol condensation.

PART IV- Viva voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4^{th} Edn., Pearson Education India, 2009.

[4] R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogels Text Book of Practical Organic Chemistry, 5^{th} Edn., Prentice Hall, 1989.

[6] R.K Bansal, Laboratory Manual of Organic Chemistry, 5^{th} Edn., New Age Publishers, 2013.

[7] N.K.Vishnoi, Advanced Practical Organic Chemistry, 3^{rd} Edn., Vikas Publishing House, 2009.

[8] J.B. Cohen, Practical Organic Chemistry, Mc Graw Hill.

[9] C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson.

[10] P.D.L Lampman and Chriz, Introduction to Organic Laboratory Techniques, College publishing.

[11] Monograph on green laboratory experiments, DST, Govt of India.

[12] http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi.

PG2CHE P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
   a) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.

3. Determination of the composition of two liquids by surface tension measurements.

Part B

Computational Chemistry Experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

[2] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

[3] J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

[4] GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html.

SEMESTER 3

PG3CHE C09 INORGANIC CHEMISTRY- III

(SOLID STATE CHEMISTRY)

Credits: 4 **Contact Lecture Hours: 72**

Module 1: Solid State Chemistry (18 Hrs)

1.1 Structure of solids: Imperfections in solids-point defects, line defects and plane defects. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), A_mX_2 (Nickel Arsenide), ABX_3 (Perovskite, Ilmenite). Spinels. Inverse spinel structures.

1.2 Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid- Type I reactions, Type II reactions.

1.3 Phase transition in solids: classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition. Kinetics of phase transitions, sintering. Growing single crystals-crystal growth from solution, growth from melt and vapour deposition technique.

Module 2: Electrical, Magnetic and Optical Properties (18 Hrs)

2.1 Free electron theory and MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Mobility of charge carriers. Hall Effect. Pyroelectricity, piezo electricity and ferro electricity. Conductivity of pure metals.

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.

2.3 Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties

2.4 Super conductivity- Type I and Type II superconductors, Frolich diagram, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates - YBaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.

Module 3: Inorganic Rings, Cages and Clusters (18 Hrs)

3.1 Ring silicates and silicones, phosphorous-nitrogen compounds, phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds. Polythiazil-one dimensional conductors

3.2 Cages: synthesis, structure and bonding of cage like structures of phosphorous. Boron cage compounds- Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes

3.3. Metal clusters: dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Module 4: Organometallic Polymers (9 Hrs)

Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Module 5: Chemistry of Materials (9 Hrs)

Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramic structures - mechanical properties, clay products, refractories- characterizations, properties and applications.

References

[1] L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.

[2] A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.

[3] D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.

[4] D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.

[5] C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.

[6] B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.

[7] A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.

[8] J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Pub.,1993, 33.

[9] F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999.

[10] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

[11] P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Pub., 2006.

[12] C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B.S. Pub., 2006.

[13] B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.

PG3CHE C10 ORGANIC CHEMISTRY - III

(ORGANIC SYNTHESES)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Retrosynthetic Analysis (9 Hrs)

1.1 Basic principles and terminology of retrosynthesis. Important strategies of retrosynthesis. Functional group interconversion. Umpolung. Synthesis of aromatic compounds. One group C-X disconnections of carbonyl derivatives and alkyl halides. Two group C-X disconnections- 1,1-, 1,2- and 1,3-difunctionalised compounds. One group C-C disconnections of alcohols and carbonyl compounds. Two group C-C disconnections- 1,2- and 1,3-difunctionalised compounds.

1.2 Amine synthesis: Primary amine, other routes to amines using reduction, reagents for the synthon NH_2^-. Alkene synthesis- from alcohols and derivatives, Wittig reaction.

Module 2: Organometallics (9 Hrs)

Preparation and applications in organic synthesis of (i) Organo lithium compounds and addition to −C=O, −COOH and –$CONR_2$ (ii) Lithium dialkylcuprates (Gilman reagent) and reaction with alkyl halides, aryl halides and enones (iii) Alkynyl Cu(I) reagents and Glaser coupling (iv) Dialkyl cadmium compounds and (v) Benzenetricarbonyl chromium and reaction with carbanions.

Module 3: Organic Synthesis via Oxidation and Reduction (18 Hrs)

3.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, Aluminium and Silver based reagents) (b) alkenes to epoxides (peroxides/per acids based)- Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to diols (Manganese and Osmium based)- Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and Lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage hydroboration- oxidation, Wacker oxidation, Selenium/Chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation.

3.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel, Homogeneous: Wilkinson) (b) Metal based reductions- Birch reduction, Pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkylstannane. Meerwein-Pondorff-Verley reduction. Baker's yeast.

Module 4: Modern Synthetic Methods and Reagents (18 Hrs)

4.1. Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Noyori reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald- Hartwig, Ullmann reactions, Wohl-Ziegler reaction. Reagents such as NBS, DDQ, DCC, Gilmann reagent.

4.2. Introduction to multicomponent reactions- Three component reactions (Mannich reaction, Passerini reaction, Biginelli reaction), Four component reactions (Ugi reaction). Click reactions (elementary idea only).

Module 5: Construction of Carbocyclic and Heterocyclic Ring System (9 Hrs)

5.1. Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization. Construction of macrocyclic rings-ring closing metathesis.

5.2. Formation of heterocyclic rings: 5- and 6-membered and condensed ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, pyridine, imidazole, thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.

Module 6: Protecting Group Chemistry (9 Hrs)

6.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection. Illustration of protection and deprotection in synthesis.

6.2 Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups used in solution phase and solid phase peptide synthesis (SPPS).

6.3 Role of trimethyl silyl group in organic synthesis.

References

[1] M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.

[2] F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.

[3] S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd Edn., Wiley, 2008.

[4] V.K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 2012.

[5] I. Ojima, Catalytic Asymmetric Synthesis, 3rd Edn., John Wiley & Sons, 2010.

[6] W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.

[7] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[8] R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

[9] L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

[10] R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, 3rd Edn., Chapmann and Hall, 1993.

[11] E. J. Corey, Xue-Min Cheng, The Logic of Chemical Synthesis, Wiley, 1995.

[12] J. Zhu, Q. Wang, M. Wang (Eds), Multicomponent Reactions in Organic Synthesis, Wiley VCH, 2015.

[13] F. Rutjes, V.V. Fokin, K.B. Sharpless, Click Chemistry: In Chemistry, Biology and Macromolecular Science, Wiley, 2012.

PG3CHE C11- PHYSICAL CHEMISTRY- III

(CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Chemical Kinetics **(18 Hrs)**

1.1 Theories of reaction rates: Collision theory- steric factor, potential energy surfaces. Conventional transition state theory- Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\#}$, $\Delta H^{\#}$ and $\Delta S^{\#}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions: free radical and chain reactions, steady state treatment, Kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism, branching chains H_2-O_2, Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step- growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

1.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

1.4 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.

Module 2: Surface Chemistry **(18 Hrs)**

2.1 Surface: Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surface excess, surface tension and surface concentration, surfactants and micelles, general properties of emulsions, foam structure, aerosols, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

2.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption- BET theory and derivation of isotherm, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

2.3 Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS.

Module 3: Catalysis (9 Hrs)

3.1 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

3.2 Enzyme catalysis and its mechanism, Michaelis-Menton equation, effect of pH and temperature on enzyme catalysis.

3.3 Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer- Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

Module 4: Colloids and Macromolecules (9 Hrs)

4.1 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

4.2 Macromolecules: Molecular mass- different averages, relation between different averages, calculation of different averages, methods of molecular mass determination- osmotic pressure, viscosity, sedimentation and light scattering methods.

Module 5: Photochemistry (18 Hrs)

5.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.

5.2 Principle of utilization of solar energy, solar cells and their working.

5.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

References

[1] J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.

[2] K.J. Laidler, Chemical kinetics, 3rd Edn., Harper & Row, 1987.

[3] C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.

[4] J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.

[5] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[6] D.A. McQuarrie, J.D. Simon, Physical chemistry: A Molecular Approach, University Science Books,1997

[7] A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley & sons, 1997.

[8] K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2nd Edn., New Age International,1986.

[9] G. Aruldhas, Molecular structure and Spectroscopy, PHI Learning, 2007.

PG3CHE C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

1.3 Problems based on the above topics.

1.4 Chirooptical properties- ORD, CD, octant rule, axial haloketone rule, Cotton effect.

Module 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling. NOE and cross polarization.

3.3 Simplification of non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling, ^{19}F and ^{31}P NMR.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer. Selective Population Inversion. DEPT. Sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, Field Desorption and Electrospray Ionization. Magnetic, TOF, quadrupole and ion cyclotron mass analysers. MS^n technique. Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Module 5: Structure Elucidation Using Spectroscopic Techniques (9 Hrs)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

[1] D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.

[2] A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.

[3] L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.

[4] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

[5] D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.

[6] H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.

[7] R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectroscopic Identification of Organic Compounds, 8th Edn., Wiley, 2015.

[8] D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008.

[9] W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.

[10] F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press,2005.

[11] E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

[12] Online spectral databases including RIO-DB.

[13] P.S. Kalsi. Spectroscopy of Organic Compounds, 5th Edn., New Age International, 2004.

SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

PG4CHE E01 INORGANIC CHEMISTRY - IV

(ADVANCED INORGANIC CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Applications of Group Theory (36 Hrs)

1.1 Transformation properties of atomic orbitals, hybridization schemes for σ and π bonding with examples, Symmetry Adapted Linear Combination of Atomic orbitals in tetrahedral, octahedral and sandwich complexes.

1.2 Ligand field theory-splitting of d orbitals in different environments using group theoretical considerations, construction of energy level diagrams, correlation diagrams, method of descending symmetry, formation of symmetry adapted group of ligands, M.O. diagrams, splitting terms for orbitals, energy levels, d-d transition-selection rules, vanishing integrals. IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

Module 2: Inorganic Spectroscopic Methods (9 Hrs)

2.1 Infrared and Raman Spectroscopy: structural elucidation of coordination compounds containing the following molecules/ions as ligands- NH_3, H_2O, CO, NO, OH^-, SO_4^{2-}, CN^-, SCN^-, NO_2^- and X^- (X=halogen).

2.2 Electron Paramagnetic Resonance Spectroscopy: EPR of d^1 and d^9 transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.

2.3 Mössbauer Spectroscopy: applications of Mössbauer spectroscopy in the study of Fe(III) complexes.

Module 3: Inorganic Photochemistry (9 Hrs)

3.1 Excited states, ligand field states, charge-transfer states and phosphorescence and fluorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications- synthesis and catalysis, chemical actinometry and photochromism. Metal-metal multiple bonds.

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

Module 4: Nanomaterials **(18 Hrs)**

4.1 General introduction to nanomaterials and emergence of nanotechnology, Moore's law, Graphene (elementary idea only), synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum, techniques of synthesis-electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films-chemical vapour deposition and atomic layer deposition techniques.

4.2 Diversity in nanosystems: self-assembled monolayers on gold-growth process and phase transitions. Gas phase clusters- formation, detection and analysis. Quantum dots- preparation, characterization and applications. Nanoshells- types of systems, characterization and application.

4.3 Evolving interfaces of nanotechnology- nanobiology, nanosensors, nanomedicines.

Module 5: Analytical Methods **(18 Hrs)**

5.1 The basis and procedure of sampling-crushing and grinding, gross sampling. Sampling of solids, liquids, gas, particulate solids, metals and alloys. Preparation of a laboratory sample. Moisture in samples- essential and non-essential water, occluded water. Determination of water in samples- direct and indirect methods.

5.2 Decompositions and dissolution-reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$ and HF. Microwave decompositions, combustion methods. Uses of fluxes like Na_2CO_3, Na_2O_2, KNO_3, $K_2S_2O_7$, NaOH, B_2O_3 and lithium meta borate.

5.3 Elimination of interferences from samples by precipitation, electrolytic precipitation, separation by extraction and ion exchange separation.

5.4 Analytical procedures involved in the environmental monitoring of water quality- BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: sampling and collection of air pollutants-SO_2, NO_2, NH_3, O_3, and PMM.

References

[1] F.A. Cotton, Chemical Applications of Group Theory, Wiley-Interscience, 1990.

[2] V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Pub., 1985.

[3] A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010.

[4] K. Nakamoto, IR and Raman Spectra of Inorganic and Coordination Complexes, Part A-Theory and Applications in Inorganic Chemistry, 6^{th} Edn., John Wiley & Sons, 1997.

[5] R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

[6] R.L. Dutta, A. Syamal, Elements of Magnetochemistry, Affiliated East-West Press, New Delhi, 1993.

[7] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4^{th} Edn., Tata McGraw Hill, 1994.

[8] A. K. Bridson, Inorganic Spectroscopic Methods, Oxford University Press, 1998.

[9] D.M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, 1994.

[10] A.W. Adamson, P.D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, 1975.

[11] V. Balzani, V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, 1970.

[12] T. Pradeep, Nano: The Essentials, Tata Mc Graw Hill, 2007.

[13] C.N.R. Rao, A. Govindaraj, Nanotubes and Nanowires, Royal Society of Chemistry, 2011.

[14] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8^{th}Edn., Saunders College Pub., 2007.

[15] J.G. Dick, Analytical chemistry, Mc Graw-Hill, 1973.

[16] S.E. Manahan, Environmental Chemistry, 9^{th} Edn., CRC Press, 2010.

[17] J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4^{th} Edn., Harper Collins College Pub., 1993.

[18] H.J. Emeleus, A.G. Sharpe, Modern Aspects of Inorganic Chemistry, 4^{th} Edn., ELBS, 1973.

[19] K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

PG4CHE E02 ORGANIC CHEMISTRY - IV

(ADVANCED ORGANIC CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Molecular Recognition and Supramolecular Chemistry (18 Hrs)

1.1 Concept of molecular recognition, host-guest complex formation, forces involved in molecular recognition.

1.2 Molecular receptors: cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes, carbon nanocapsules.

1.3 Importance of molecular recognition in biological systems like DNA and protein. Controlled release phenomena.

1.4 Applications of supramolecular complexes in perfumery and medicine. Targeted drug delivery.

Module 2: Green Alternatives to Organic Synthesis (9 Hrs)

2.1 Principles of Green Chemistry: basic concepts, atom economy, twelve principles of Green Chemistry, principles of green organic synthesis.

2.2 Green alternatives to Organic Synthesis: coenzyme catalyzed reactions, thiamine catalyzed benzoin condensation. Green alternatives of molecular rearrangements: pinacol-pinacolone and benzidine rearrangements. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalyzed synthesis. Condensation reactions. Green photochemical reactions.

2.3 Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry.

2.4 General principles of microwave and ultrasound assisted organic synthesis.

Module 3: Chromatrographic techniques (9 Hrs)

Chromatographic techniques: theory of chromatography, Applications of adsorption, partition, paper, thin layer and column chromatographic methods. LC, HPLC, IEC, GC and GPC. Column matrices. Detectors. Affinity and chiral columns.

Module 4: Stereoselective Transformations (9 Hrs)

4.1 Asymmetric induction-chiral auxiliaries and chiral pool.

4.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

4.3 Asymmetric aldol condensation pioneered by Evans.

4.4 Asymmetric Diels-Alder reactions.

4.5 Asymmetric epoxidation using Jacobsen's catalyst.

Module 5: Chemistry of Natural Products and Biomolecules - I (18 Hrs)

5.1 Steroids: Classification and nomenclature of steroids. Basic principles of the biosynthesis of steroids. Reactions, structure elucidation, stereochemistry and biosynthesis of cholesterol. Structure and semisynthesis of steroid hormones- testosterone, estrogen. Biomimetic synthesis of progesterone.

5.2 Alkaloids: Classification of alkaloids. General methods of structure elucidation of alkaloids. Structure elucidation and synthesis of papaverine, quinine and morphine. Basic principles of the biosynthesis of alkaloids. Biosynthesis of morphine. Biogenesis of alkaloids. Biomimetic synthesis of spatriene.

5.3 Terpenoids: Classification of terpenoids. Synthesis of camphor. Basic principles of the biosynthesis of terpenes. Biosynthesis of α-terpineol. Biogenesis of isoprenoids.

5.4 Carbohydrates: Classification of carbohydrates. Basic principles of the biosynthesis of carbohydrates. Biosynthesis of glucose.

5.5 Plant pigments: Anthocyanins and carotenoids. Structure and synthesis of cyanin, flavones, quercetine and β-carotene.

5.6 Lipids: Classification of lipids.

Module 6: Chemistry of Natural Products and Biomolecules - II (9 Hrs)

6.1 Vitamins: Classification of vitamins. Structure of vitamins A, B_1, B_2, B_6 and C. Synthesis of vitamins A, B_1, B_2 and C.

6.2 Amino acids, proteins and nucleic acids: Classification. Basic principles of the biosynthesis of proteins and nucleic acids. Biosynthesis of phenyl alanine. Primary, secondary, tertiary and quarternary structure of proteins. Methods for primary structure determination of peptides, proteins and nucleic acids. Replication of DNA, flow of genetic information, protein biosynthesis, transcription and translation,

Genetic code, regulation of gene expression, DNA sequencing. The Human Genome Project. DNA profiling and the Polymerase Chain Reaction (PCR).

6.3 Prostaglandins: Nomenclature. Synthesis of PGE_2 and PGF_2.

Module 7: Medicinal Chemistry and Drug Designing (9 Hrs)

7.1 Introduction to Drug design:-Drug action, receptor theories, receptor proteins, drug receptor interaction, drug metabolism-different pathways. Combinatorial synthesis and modeling techniques (a brief study).

7.2 Important drugs used in the following classes with mode of action:-. Antibacterial agents (Penicillins, cephalosporins, tetracyclines, chloramphenicol, ciprofloxacin, isoniazid), Antiparasitic agents (Ivermectin), Analgesics (Aspirin), Antiviral agents (Acyclovir, oseltamivir), Anticancer agents (podophyllotoxin, calicheamicin, tamoxifen, paclitaxel), CNS Drugs (Salbutamol, Ephedrine, Phenobarbital), Antisyphilitic agents (Salvarsan), Cholesterol lowering agents (Lovastatin), Immunosuppressants (cyclosporine), Vasodialators (Viagra), Narcotics (Methadone).

7.3 Applications of nanomaterials in medicine.

Module 8: Advances in Polymer Chemistry (9 Hrs)

8.1 Conducting polymers, polymers for NLO applications, temperature resistant and flame retardant polymers, polymers for medical applications.

8.2 Dendrimers and dendritic polymers: terminology, classification of dendrimers. Methods of synthesis: convergent and divergent approaches. Dendrimers as nanocapsules. Applications of dendrimers as organo catalysts. Hyper branched polymers: definition, examples, synthesis and applications.

References

[1] J.M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, 1995.

[2] F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, 1993.

[3] Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

[4] V.K. Ahluwalia, Green Chemistry, Ane Books, 2009.

[5] T. Pradeep, Nano: the Essentials, Tata McGraw Hill, 2007.

[6] W. Carruthers, I.Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2004.

[7] J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

[8] R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, Blackie Academic and Professional, 1993.

[9] J.M. Berg, J.L. Tymoczko, L. Stryer, Biochemistry, 6th Edn., W.H. Freeman,2010.

[10] A.L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, 5th Edn., W.H. Freeman, 2008.

[11] V.K. Ahluwalia, M. Chopra, Medicinal Chemistry, Ane Books, 2008.

[12] V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, CRS Press, 2007.

[13] S.V. Bhat, B.A. Nagasampagi, M. Sivakumar, Chemistry of Natural Products, Springer Science & Business Media, 2005.

[14] P. S. Kalsi, S. Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Alpha Science, 2013.

[15] T. Nogrady, D. F. Weaver, Medicinal Chemistry: A Molecular and Biochemical Approach, 3rd Edn., Oxford University Press Inc., 2005.

[16] D. Sriram, P. Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.

[17] K . D. Tripathi, Essentials of Medical Pharmacology, 6th Edn., Jaypee, 2008.

[18] P. Chandrasekhar, Conducting Polymers, Fundamentals and Applications: A Practical Approach, Springer Science & Business Media, 2013.

PG4CHE E03 PHYSICAL CHEMISTRY - IV

(ADVANCED PHYSICAL CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Crystallography **(18 Hrs)**

1.1 Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.

1.2 Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.

1.3 Liquid crystals: mesomorphic state, types, examples and applications of liquid crystals. Theories of liquid crystals. Photoconductivity of liquid crystals.

Module 2: Electrochemistry **(18 Hrs)**

2.1 Conductance measurements, results of conductance measurements, ionic mobilities, influence of pressure and temperature on conductance of ions, Walden equations, abnormal ionic conductance.

2.2 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye- Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL. Osmotic coefficient, ion association, fraction of association, dissociation constant, triple ion and conductance minima, equilibria in electrolytes.

2.3 Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties.

Module 3: Electrode Double layer and Polarisation (9 Hrs

3.1 Electrode double layer, electrode-electrolyte interface, different models of double layer-Helmholtz compact layer model, Guoy-Chapman model, Stern model, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential.

3.2 Fuel cells, classification based on working temperature, chemistry of fuel cells, H_2-O_2 fuel cells.

3.3 Polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, theories of overvoltage, Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants.

Module 4: Quantum Statistics (9 Hrs)

4.1 Need for quantum statistics, Bose-Einstein statistics, Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi-Dirac distribution, examples of particles, application in electron gas, thermionic emission. Comparison of three statistics- Maxwell Boltzmann, Bose Einstein and Fermi - Dirac Statistics.

4.2 Heat capacity of solids- Dulong and Petit's law, the vibrational properties of solids, Einsteins theory- derivation and its limitations. Debye theory – derivation and its limitations.

Module 5: Electroanalytical Techniques (18 Hrs)

5.1 Voltametry and polarography: Voltametry-cyclic voltametry, ion-selective electrodes, anodic stripping voltametry. Polarography- decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves, the dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition method, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.

5.2 Amperometric titrations: General principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, instrumentation, titration procedure, merits and demerits of amperometric titrations.

5.3 Coulometry: Coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric titrations, applications of coulometric titrations- neutralization titrations, complex formation titrations, redox titrations. Advantages of coulometry.

Module 6: Diffraction Methods, Atomic Spectroscopic Techniques and Fluorescence Spectroscopy (18 Hrs)

6.1 Electron diffraction of gases. Wierl's equation. Neutron diffraction method. Comparison of X-ray, electron and neutron diffraction methods.

6.2 Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.

6.3 Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.

6.4 Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation.

6.5 Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorophores: long life time metal-ligand complexes.

References

[1] L.V. Azaroff, Introduction to Solids, McGraw Hill, 1984.

[2] D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.

[3] R.J. Silbey, R.A. Alberty, M.G. Bawendi, Physical Chemistry, 4^{th} Edn., Wiley, 2005.

[4] G.M. Barrow, Physical Chemistry, 5^{th} Edn., Tata McGraw Hill, 2007.

[5] A.R. West, Basic Solid State Chemistry, John Wiley & Sons, 1999.

[6] K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.

[7] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[8] G.W. Castellan, Physical Chemistry, Addison-Wesley, 1983.

[9] B. Valeur, Molecular Fluorescence: Principles and Applications, Wiley-VCH 2002.

[10] J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd Edn., Springer, 2006.

[11] D.L. Andrews, A.A. Demidov, Resonance Energy Transfer, Wiley, 1999.

[12] S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, 2011.

[13] D.R. Crow, Principles and Applications of Electrochemistry, 4th Edn., CRC Press, 1994.

[14] B.K. Sharma, Electrochemistry, Krisna Prakashan, 1985.

[15] H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.

[16] A.I. Vogel, A Text Book of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, 1961.

[17] H.H. Willard, J.A .Dean, L.L. Merritt, Instrumental Methods of Analysis, Van Nostrand, 1965.

[18] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

[19] R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, TataMcGraw Hill,1999.

[20] Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall, 2002.

[21] F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975.

[22] J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971.

PG4CHE E04 - POLYMER CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Introduction to Polymer Science (9 Hrs)

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization (18 Hrs)

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

2.2 Ionic polymerization, common features of two types of ionic polymerization, mechanism and kinetics of cationic polymerization, expressions for overall rate of polymerization and the number average degree of polymerization, mechanism and kinetics of anionic polymerization, expressions for overall rate of polymerization and the average degree of polymerization, living polymers.

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

2.4 Copolymerization, types of copolymers, the copolymer composition equation, reactivity ratio and copolymer structure-influence of structural effects on monomer reactivity ratios, the Q-e scheme, synthesis of alternating, block and graft copolymers.

2.5 Step reaction (condensation) polymerization, Carothers equation, mechanism of step reaction polymerization, kinetics of step reaction polymerization, number distribution and weight distribution functions, polyfunctional step reaction polymerization, prediction of gel point.

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability- mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications.

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

7.1 Basic concepts and terminology: Dendrons, star shaped and star bust polymers, dendrimer formation and generations, various types of dendrimers.

7.2 Synthesis of dendrimers- convergent and divergent approaches, methods and mechanism. Properties of dendrimers- polydispersity, mechanical properties, viscoelastic properties. Determination of physical properties.

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (^{1}H and ^{13}C NMR), mass spectral studies (MALDI and TOF).

7.4 Dendritic macromolecules: hypergrafted and hyperbranched polymers - definition and classification, synthesis-methods and mechanism, characterization, properties, applications

References

1. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

2. F.W. Billmeyer Jr., Textbook of Polymer Science, 3rd Edn., Wiley-India, 2007.
3. L. H. Sperling, Introduction to Physical Polymer Science, 4th Edn, John Wiley & Sons, 2006.
4. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2008.
5. D.I. Bower, An Introduction to Polymer Physics, Cambridge University Press, 2002.
6. M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving approach, CRC/Taylor & Francis, 2006.
7. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1983.
8. J.R. Fried, Polymer Science and Technology, 2nd Edn., Prentice Hall, 2003.
9. G. Odian, Principles of Polymerization, 4th Edn., John Wiley & Sons, 2007
10. K.J. Saunders, Organic Polymer Chemistry, Chapmann & Hall, 1973.
11. K. Matyjaszewski, T.P. Davis, Handbook of Radical Polymerization, John Wiley & Sons, 2003.
12. H.R. Allock, F. W. Lampe, Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003.

PG4CHE E05 ANALYTICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Instrumental Methods **(36 Hrs)**

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods-precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio, hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments- sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentrationelectron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry- magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{32}P). Principle of MRI.

Module 2: Sampling **(18 Hrs)**

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non essential water, absorbed and occluded water, determination of water (direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples - separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Module 3: Applied Analysis (9 Hrs)

3.1 Analytical procedures involved in environmental monitoring. Water quality- BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil-moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Module 4: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

4.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection (indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

4.2 Capillary electro chromatography- packed columns. Micellar electro kinetic chromatography.

Module5: Process instrumentation (9 Hrs)

5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Module 6: Aquatic Resources (9 Hrs)

6.1 Aquatic resources: renewable and non renewable resources, estimation, primary productivity and factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea- extraction and recovery of chemicals, salt from solar evaporation.

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

[2] D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8^{th} Edn., Saunders College Pub., 2007.

[3] R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.

[4] H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.

[5] G.D. Christian, J.E. O’Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

[6] J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

[7] J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.

[8] E.D. Howe, Fundamentals of Water Desalination, M. Dekker, 1974.

SEMESTERS 3 AND 4

PG4CHE P04– INORGANIC CHEMISTRY PRACTICAL – 2

Credit: 3 **Contact Lab Hours: 54 + 54 = 108**

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, illmenite.

References

[1] A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.

[2] I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.

[3] G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.

[4] N.H. Furman, Standard Methods of Chemical Analysis: Volume 1, Van Nostrand, 1966.

[5] F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub., 2006.

PG4CHE P05 ORGANIC CHEMISTRY PRACTICAL-2

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

A. Volumetric estimation of 1) Aniline 2) Phenol 3) glucose 4) Iodine value and saponification value of oil

B. Spectrophotometric/colorimetric estimation of 1) Aniline 2) Glucose 3) Cholesterol 4) ascorbic acid 5) Streptomycin 6) Aspirin.

PART II

Preparation of compounds by two stages.

1) Acetanilide – p-nitroacetanilide – p-nitroaniline
2) Methyl benzoate – m-nitromethylbenzoate – m-nitrobenzoic acid
3) Acetanilide – p-bromoacetanilide – p-bromoaniline
4) Phenol – salicylaldehyde – coumarin
5) Benzophenone – benzophenone oxime – benzanilide
6) Aniline – 2,4,6-tribromoaniline – 1,3,5-tribromoaniline
7) Benzaldehyde-benzoin-benzilic acid
8) Aniline-sulphanilic acid-methylorange
9) O-Toluidine-o-methyl acetanilide-N-acetyl anthranilic acid
10) Aniline-acetanilide-p-nitroacetanilide

PART III

Enzyme/coenzyme catalyzed reactions.

PART IV

Preparation Involving Green Alternatives of Chemical Methods.

PART V

Microwave assisted Organic Synthesis.

PART VI

Prediction of FTIR, UV-Visible, ^{1}H and ^{13}C NMR spectra of the substrates and products at each stage of the products synthesized by the above methods.

PART VII – Viva - voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

[4] J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

[6] Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

[7] R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectroscopic Identification of Organic Compounds, 8th Edn., Wiley, 2015.

[8] F. G. Mann and B.C. Saunders, Practical Organic Chemistry, Pearson Education India, 2009.

[9] J. B. Cohen, Practical Organic Chemistry, McGraw Hill.

[10] C.E Bella and D.F Taber, Organic Chemistry laboratory, Thomson.

[11] P.F Shalz, J. Chem. Education, 1996, 173, 267.

[12] P.D.L Lampman and Chriz, Introduction to Organic Laboratory techniques, College publishing.

[13] http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

PG4CHE P06 PHYSICAL CHEMISTRY PRACTICAL-2

Credit: 3 **Contact Lab Hours: 72+72=144**

I Chemical Kinetics

1. Determination of the rate constant of the acid / alkaline hydrolysis of ester.
2. Determination of Arrhenius parameters.
3. Kinetics of reaction between $K_2S_2O_8$ and KI
4. Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI
5. Iodination of acetone in acid medium.

II Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution.
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

III Refractometry

1. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water).
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

IV Viscosity

1. Determination of viscosity of pure liquids.
2. Verification of Kendall's equation.
3. Determination of the composition of binary liquid mixtures (alcohol-water, benzene-nitrobenzene).
4. Determination of the molecular weight of a polymer (polystyrene in toluene).

V Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pKa values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a mixture of acids against a strong base.
6. Titration of a dibasic acid against a strong base.

VI Potentiometry

1. Determination of single electrode potentials (Cu and Zn).
2. Application of Henderson equation.
3. Titrations.
4. Determination of end point of a titration using Gran Plot.
5. Determination of the concentration of a mixture of Cl^- and I^- ions.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

[2] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

[3] B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005.

M.Sc. Degree Chemistry Programme

Aim and Objective of the Syllabi

Aim
Chemistry is a central subject of science. It is also closely related to daily life. The Master's program not only offers the option of focusing on a specialist area but students will also acquire the necessary skills for this and they will learn to think independently and act responsibly. Graduates will become familiar with the terminologies and special aspects of chemistry, its strengths and limitations and will be able to apply their knowledge to new issues and situations, even in an interdisciplinary context. They will gain knowledge and practical skills relating to the current state of research in selected fields. They will be able to analyze chemical issues and assess them critically, to develop independent solution strategies and to estimate their impacts in a wider context. The broad spectrum of the academic program will ensure that students acquire the skills necessary for demanding fields of activity in industry, economy and administration

Objective
The Master's course in chemistry is designed with an objective to teach post graduates with the skills to critically assess and deal with issues requiring the utilization of chemical principles from each sub-disciplines such as organic, inorganic, physical, analytical and biochemistry. It is the objective of the chemistry program to teach students the necessary knowledge in a way that enables them to familiarize themselves quickly with new developments, to be introduced to new areas and to make independent contributions to further developments of research and technology in their specialized area once they have finished their program.

Semester 1

PG1CHE C01 Inorganic Chemistry - I

Aims and Objectives
This is a chemistry module designed for chemistry majors and features the principles of coordination chemistry, boron compounds and that of nuclear chemistry. In depth discussion about coordination compounds focusing primarily on their structure and various aspects of bonding will be done. The course covers synthesis, structure and bonding of organometallic compounds. Kinetics of reactions of metal complexes and their mechanism will also be illustrated. The learners should be able to apply these topics in various fields.

- To mould the chemistry majors in coordination chemistry, boron compounds and nuclear chemistry
- To understand the structure and various aspects of bonding in the coordination compounds
- To achieve knowledge about the synthesis, structure and bonding of organometallic compounds
- To illustrate the kinetics of reactions and their mechanism of metal complexes
- To acquire ability to apply the theoretical knowledge in various fields

PG1CHE C02 Organic Chemistry - I

Aims and Objectives

The module deals primarily with the basic principles to understand the structure and reactivity of organic molecules. Emphasis is on substitution and elimination reactions of aliphatic and aromatic compounds. Learners will get the essential ideas on how simple molecules can be constructed. Bonding in conjugated systems, reactions mechanism, organic transformations and stereochemistry will likewise be discussed.

- To understand the structure and reactivity of organic molecules
- To emphasize the substitution and elimination reactions of aliphatic and aromatic compounds
- To get an idea about the construction of simple organic molecules
- To impart knowledge about stereochemistry of organic compounds and basic principles of conformational analysis
- To know the bonding in conjugated systems and various reaction mechanisms

PG1CHE C03 Theoretical Chemistry - I

Aims and Objectives

This module looks at quantum chemistry and group theory. A more profound comprehension of quantum chemistry beginning from its postulates and basic systems such as particle-in-a-box to hydrogen like atoms is explored. The second part of the module looks at molecular symmetry and applications in molecular orbitals analysis and vibrational spectroscopy, electronic transitions of carbonyl chromophore and origin of selection rule of electronic transition. Learners will be able to apply these ideas to individual atoms and molecular systems.

- To get a comprehensive idea about quantum chemistry and group theory
- To discuss the emergence of classical mechanics over quantum mechanics
- To get an awareness about the basic postulates of quantum chemistry and its application to hydrogen and hydrogen like atoms
- To acquire knowledge for deriving the wave function, energy, momentum etc. of a particle under different conditions of motions
- To impart knowledge about the molecular symmetry and its applications in molecular orbitals analysis
- To gain information about various spectroscopic techniques, their selection rules and applications based on group theory
- To solve the problems based on the theories

PG1CHE C04 Physical Chemistry - I

Aims and Objectives

Physical chemistry is the study of phenomena in chemical systems in terms of physical concepts and laws. In this module, different branches of thermodynamics will be explored. In *Classical Thermodynamics* kinetic theory of gases, and the energetics of chemical reactions will be explored. Thermodynamics of natural processes and energy transformations in living organisms will be discussed in *Irreversible thermodynamics*. *Statistical Thermodynamics* looks at the relationship between molecular and bulk properties of matter, including examples such as the use of partition functions in equilibrium, transition states and heat capacity of chemical systems. Learners will be familiarized with the behavior of matter in bulk.

- To study the different phenomena in chemical systems in terms of physical concepts and laws
- To analyze different branches of thermodynamics like *Classical Thermodynamics, Irreversible thermodynamics* and *Statistical Thermodynamics*
- To explore the kinetic theory of gases and the energetics of chemical reactions
- To discuss thermodynamics of natural processes and energy transformations in living organisms
- To correlate the molecular and bulk properties of matter, including partition functions in equilibrium, transition states and heat capacity of chemical systems
- To familiarise the behaviour of matter in bulk
- To solve the problems based on the theories

Semester 2

PG1CHE C05 Inorganic Chemistry - II

Aims and Objectives
This module covers three parts: non-aqueous solvents, bioinorganic chemistry and organometallic chemistry. Part 1 deals with acid-base concept and reactions in non-aqueous solvents. Part 2 describes basic principles and concepts of bioinorganic chemistry including the mechanisms of reactions catalyzed by metalloproteins, and kinetics of electron transfer in proteins. Part 3 focusses on the spectral and magnetic properties of transition metal complexes. A comprehensive discussion on inorganic cages and metal clusters follows. The learners will understand the different modes of reactions of organometallic compounds and their applications can be explored.

- To understand the basic concepts and principles of bioinorganic chemistry
- To familiarise the mechanisms and kinetics of different reactions catalysed by metalloenzymes
- To explore the electronic spectra and magnetic properties of transition metal complexes
- To study the stereochemistry of coordination compounds
- To understand the different reactions and catalysis of organometallic compounds

PG1CHE C06 Organic Chemistry - II

Aims and Objectives
This module covers the study of a selected series of organic reactions involving reactive intermediates and/or molecular rearrangements. Emphasis is placed on an understanding of their reaction mechanisms. These will include reactions involving carbocations, carbanions, carbenes, carbenoids, nitrenes and arynes as intermediates. Reactions initiated by radicals will be covered. Comprehensive discussions on organic photochemistry including the rules and stereochemical consequences in pericyclic reactions will be given. The learners should be able to apply these ideas in the field of organic synthesis.

- To understand the basic concepts of selected series of organic reactions involving reactive intermediates and/or molecular rearrangements
- To acquire knowledge about name reactions involving radical intermediates
- To understand the symmetry properties of molecular orbitals of selected compounds
- To develop idea about pericyclic reactions
- To understand the basic principles of photochemistry and to apply these principles in different photochemical reactions

PG2CHE C07 Theoretical Chemistry - II

Aims and Objectives

The objective of this model is to familiarize the learner with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding. Molecular structure evaluation using group theory will enable the learners to apply it in the field of spectroscopy. To apply the concept of molecular modelling to isolated molecular systems.

- To get idea about various approximation methods to solve many electron systems other than simple systems.
- To discuss the applications of variation method and perturbation method for He atom
- To get an awareness about the SCF, HFSCF methods etc.
- To acquire ability to solve Schrödinger equations for molecules.
- To familiarize with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding.
- To acquire ability to apply MO treatment to homo and heteronuclear molecules
- To impart knowledge about the HMO theory and its applications to various molecules
- To evaluate molecular structure by using group theory
- To gain information about computational chemistry as a tool and find its applications
- To familiarize different molecular mechanics methods and to understand different force fields
- To achieve knowledge about different methods like HF, Ab initio, molecular mechanics semiempirical, DFT etc.
- To acquire ability to write the Z matrix of different type of molecules
- To familiarize about GAMESS/Firefly and its applications
- To solve the problems based on the theories

PG2CHE C08 Physical Chemistry - II

Aims and Objectives

In this module, the basic idea of how light interacts with matter, in particular atoms and molecules will be conferred. Microwave, infrared, Raman, electronic and nuclear magnetic resonance spectroscopic techniques will be discussed. Students will be able to apply these principles in the area of molecular spectroscopy.

- To understand the origin of different spectra and characterise the regions of the electromagnetic spectrum.
- To familiarise the microwave spectroscopy and its applications
- To identify Morse potential energy diagram and different types of bands and different types of vibrations and the application of IR spectroscopy
- To get aware about FT spectroscopy and FTIR
- To characterize term symbols and electronic spectra of different molecules
- To identify different types of lasers and realise its applications
- To understand the Mossbauer spectroscopy by learning the principle and recording of spectrum including Doppler effect, chemical shift etc.
- To familiarise the Raman spectroscopy and its applications
- To interpret the complementarities of Raman and IR spectra
- To understand the basic principles of NMR spectroscopy
- To familiarise the second order effects on spectra

- To understand NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR,
- To familiarise EPR and NQR spectroscopy

PG2CHE P01 Inorganic Chemistry Practical - I

Aims and Objectives
This is a module intended for chemistry majors. It deals with qualitative and quantitative inorganic analysis along with preparation and characterization of inorganic complexes. The learners will have the option to apply these ideas in various fields pertaining to inorganic chemistry.

- To familiarise different metal salts including rare earths
- To analyse quantitatively different ions using colorimetry
- To characterize the synthesised inorganic complexes

PG2CHE P02 Organic Chemistry Practical - I

Aims and Objectives
In this module, students will learn to apply various techniques to separate a mixture into its individual components and identify each component. Guided under the general principles of analytical and physical chemistry, these techniques include solvent extraction, TLC and column chromatography. Students will also acquire the skill to use the computational tools to draw the reaction schemes and mechanisms of various organic reactions.

- To develop skill in separating different organic mixtures and analyse it
- To familiarise various separation techniques such as solvent extraction, TLC and column chromatography
- To acquire skill to draw structure of organic compounds and the reaction schemes and mechanism of organic reactions using Chemsketch

PG2CHE P03 Physical Chemistry Practical - I

Aims and Objectives
In this module, students will learn about the practical applications of various principles of physical chemistry like phase rule, adsorption, and surface tension. Learners will be able to use computational software to predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy, and predict its spectral behavior.

- To familiarise different isotherms and to determine the concentration of the given acid using the isotherms
- To construct the phase diagrams of simple eutectics and three component systems
- To acquire knowledge about the effect of salts on miscibility temperature
- To calculate distribution coefficient and equilibrium constant based on distribution law
- To determine the surface tension of a liquid by various methods
- To acquire knowledge about computational software like GAMESS/Firefly

- To predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy by using GAMESS/Firefly.

Semester 3

PG3CHE C09 INORGANIC CHEMISTRY- III (SOLID STATE CHEMISTRY)

- To get an understanding about the structure of solids, defects in solids and different solid state reactions
- To discuss the electrical, magnetic and optical properties in the solid state
- To study different types of cage, ring and cluster compounds in inorganic systems
- To acquire some knowledge about different types of organometallic polymers
- To understand the chemistry, properties and applications of different inorganic materials in chemistry

PG3CHE C10 Organic Chemistry-III (Organic Synthesis)
Aim:

Course Objectives:

- To identify the basic principles, terminology and important strategies of retro synthesis
- To make awareness about the reagents and basic organic reactions
- To understand the chirality, chiral catalyst and asymmetric synthesis
- To study the influence of light and thermal energy for the formation of cyclic systems
- To aware of basic ideas and applications of supramolecular chemistry
- To understand the structure determination and synthesis of natural products

Course Outcomes:

- To identify the basic principles, terminology and important strategies of retro synthesis
- To make awareness about the reagents and basic organic reactions
- To study the influence of light and thermal energy for the formation of cyclic systems
- To aware of basic ideas and applications of supramolecular chemistry
- To understand the structure determination and synthesis of natural products
-

- To enable the students to use retrosynthetic analysis for the construction of synthetic routes for simple organic compounds and logical dissection of complex organic molecule and to use advanced synthetic methodology in preparing organic compounds.
- To know and understand the reactivity of organometallic compounds including their application in synthesis. Knowledge of a variety of organometallic based catalytic reactions including a mechanistic understanding.
- To enable the students to acquire proper knowledge about various methods of oxidation and reduction reagents. Students will learn about synthetically useful transformations including oxidations and reductions reactions. The emphasis will be on developing a mechanistic understanding of selectivity and synthetic strategy.

- Enable to use various reagents and organic reactions in a logical manner in organic synthesis. An ability to apply synthetic reagents like, DDQ, NBS, DCC, Gilmann reagent etc in organic synthesis and to get insights into novel reactions and reagents in organic synthesis ·
- The students will be able to understand different approached toward the synthesis of carbocyclic and heterocyclic ring formation etc.
- To impart the students in depth knowledge about the heterocyclic compounds for different elements containing heterocyclic ring and to develop quantitative ideas about the synthesis, properties and uses of such heterocyclic compounds like thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.
- To impart the students in depth knowledge about name reactions in cyclisation and construction of macrocyclic rings-ring closing metathesis.
- To know the utility of protecting group strategy in organic synthesis.
- To impart the students a thorough knowledge about Chemo and regio selective protection and deprotection.
- To Provide theoretical background about protecting groups used in solution phase and solid phase peptide synthesis (SPPS) and understand the role of trimethyl silyl group in organic synthesis.

PG3 CHE C11 Physical chemistry- III (Selected topics in Physical Chemistry)

Objectives:

- To give an in-depth account of different theories of reaction rates, kinetics of fast reactions and reaction in solution.
- To study the different types of quantum statistics and its comparison, Laws related to heat capacity of solids, phase transition and thermionic emission.
- To study the chemistry of surfaces and various techniques employed for the characterization of different types of surface phenomena and the importance of adsorption process and catalytic activity at the solid surfaces
- To impart knowledge about acid-base, enzyme and surface catalysis.
- To impart knowledge about enzyme inhibition, protein folding and molecular motors.
- To recognize the general properties of colloids and macromolecules
- To acquire knowledge of photochemistry and photophysical principles, their applications

Outcome:

- The student will acquire knowledge about different theories on reaction rate, can analyse the mechanistic path and the experimental conditions of different types of reactions.
- Will able to understand the different techniques for analysing fast reactions.
- Will able to classify the particles according to different statistics and to do problems based on the arrangement of particles in different energy states.
- To compare the different laws related to heat capacities.
- To generate idea about phase transitions and thermionic emissions.
- Will acquire knowledge about the acid base catalysis, enzyme catalysis and their principles.

- Will appreciate the applications of chemical principles of surface catalysis and colloidal chemistry in industrial synthesis.
- Able to classify colloids present in nature and apply its properties in daily life.
- Apply the principles of adsorption in daily life situations.
- The student will able to apply photochemistry and photophysical principles on environmental and biological processes and will explain photophysical energy conversion to generate electricity
- Gains numerical ability and analysing power to solve problems.

PG3CHE C12 Spectroscopic Methods in Chemistry

Course Objectives:

- To understand the basic ideas of different spectroscopic Techniques
- To identify the compounds by analyzing the UV, IR NMR and Mass spectrum
- To interpret the spectrum of organic compounds
- To develop the structure elucidation skill of organic compounds using different types of spectral data

Outcome:

- Achieve advanced knowledge about the interactions of electromagnetic radiation and matter and their applications in spectroscopy.
- To understand the selection rules of UV-Visible spectroscopy and learn the various rules to calculate the absorption maxima.
- Study the chirooptical properties and do the problems
- be able to analyse and interpret IR spectroscopic data based on stereochemistry and various factors influencing the spectra study the basic principles of NMR and factors influencing spectra and understand the advanced topics like two dimensional spectroscopy.
- Study mass spectroscopic techniques and problems based on it.
- Be able to solve problems related to the structure and to study molecular interactions by choosing suitable spectroscopic methods and interpreting corresponding data.

Semester 4

PG4CHE E01 INORGANIC CHEMISTRY - IV (ADVANCED INORGANIC CHEMISTRY)

- To apply group theory to metal complexes
- To learn the application of spectroscopic techniques to coordination complexes
- To understand the basic concepts in inorganic photochemistry and its applications
- To get introduced to nanomaterials, the emergence of nanotechnology and the diversity in nano systems
- To familiarise with the different analytical methods and procedures
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PG4CHE E02 ORGANIC CHEMISTRY – IV (ADVANCED ORGANIC CHEMISTRY)

- To get a brief idea and appreciation of the significance and application of supramolecular chemistry and its applications in organic chemistry, chemical biology, medical and perfumery industries. Based on the analysis of a series of host molecules, students able to identify and hypothesize the trends in reactivity and binding of guests.
- To learn the principles of green chemistry and to know the various green protocols in organic synthesis.
- To explain how Green chemistry and sustainability relates to problems of society, the environment, and economic development.
- To provide theoretical background and develop practical skills for analysing materials using modern analytical methods Chromatrographic techniques.
- To study the important stereoselective transformations in organic synthesis like Asymmetric induction, Enantioselective catalytic hydrogenation, Asymmetric aldol condensation, Asymmetric Diels-Alder reactions and Asymmetric epoxidation.
- To impart the students thorough idea in in the chemistry of terpenoids, steroids, alkaloids, lipids, plant pigments, vitamins, proteins and nucleic acids.
- To enable the students to understand and study nomenclature and synthesis of Prostaglandins.
- To understand the role of synthetic chemistry in the development of pharmaceutical agents and the modification of chemical structures to develop new drug molecules.
- Be able to describe the modern and innovative discovery of pharmaceuticals and applications of nanomaterials in medicine.
- To describe the key concepts and strategies used in conducting polymers, dendrimers and dendritic polymers.
- To get an overview about different kinds of polymers and its applications.

PG4CHE E03 PHYSICAL CHEMISTRY - IV (ADVANCED PHYSICAL CHEMISTRY)

Aim: This subject is designed to impart fundamental knowledge on topics like crystallography, electrochemistry, Electrode Double layer and Polarisation, Electroanalytical Techniques, Quantum Statistics, Diffraction Methods, Atomic Spectroscopic Techniques and Fluorescence Spectroscopy etc.

Objectives:

- To study different types of crystal systems and different methods of characterizing crystal structure.
- To analyse structure factor.
- To impart knowledge about Liquid crystals including mesomorphic state, types, examples, theories and applications of liquid crystals.
- To study Conductance measurements
- The objective is to study the basics of electrochemistry and its importance to modern industry and technology.
- To study the electrode double layer, different models of double layer and membrane potential.
- To study the general properties of polarization
- To study different types and theories of overvoltage.

- To study fuel cells.
- To study the different types of quantum statistics and its comparison, Laws related to heat capacity of solids, phase transition and thermionic emission.
- To understand different electroanalytical techniques like Voltametry, polarography,amperometry and colometry
- To study the Electron diffraction of gases
- To study the principle and instrumentation of various spectroscopic techniques like AAS, AES and FES
- To understand the fluorescence sensing, mechanism of sensing and the applications of novel fluorophores

Outcome:

- The student will acquire knowledge about different types of crystals systems.
- Will be able to understand structure factor.
- Will be able to understand Liquid crystals including mesomorphic state, types, examples, theories and applications of liquid crystals.
- Acquire knowledge about conductance measurements
- Understand theories of ions in solutions.
- Apply the theories to explain the variation of ionic conductance with concentration, electric field
- Will able to classify the particles according to different statistics and to do problems based on the arrangement of particles in different energy states.
- To compare the different laws related to heat capacities.
- To generate idea about phase transitions and thermionic emissions.
- The student will acquire knowledge about electrode double layer, different models of double layer and membrane potential.
- The student will acquire knowledge about polarization and different types and theories of overvoltage
- Will acquire knowledge about fuel cells.
- Will able to illustrate different electroanalytical techniques like voltametry, polarography, amperometry and colometry
- Will acquire knowledge about the fluorescence sensing, mechanism of sensing and the applications of novel fluorophores
- Gains numerical ability and analysing power to solve problems .

PG4CHE P04– INORGANIC CHEMISTRY PRACTICAL – 2

Aims and Objectives

This is a module intended for chemistry majors. It deals with quantitative inorganic analysis of simple binary mixtures of metallic ions in solution by volumetric and gravimetric methods. Includes the analysis of the alloys and ores. The learners will have the option to apply these ideas in various fields pertaining to inorganic chemistry.

- To estimate simple binary mixtures of metallic ions in solution by volumetric and gravimetric methods.
- To analyse different alloys and ores

PG4CHE P05 ORGANIC CHEMISTRY PRACTICAL - 2

- To acquire skill in estimation of various organic compounds volumetrically and colorimetrically
- To familiarise two stage preparation of organic compounds
- To develop skill in green methods for preparing organic compounds using green solvents as well as Microwave assisted Organic Synthesis.
- To develop skill for predicting the FTIR, UV-Visible, ^1H and ^{13}C NMR spectra of the substrates and products at each stage of the synthesis.

PG4CHEP06 PHYSICAL PRACTICAL – II

This course is intended to acquaint the students with the practice of physical chemistry experiments. The educational philosophy of the labs is that experimental physical chemistry has a life of its own.

Aim: This practical session deals with the fundamentals of physical chemistry experiments including Chemical Kinetics, Polarimetry, Refractometry, Viscosity, Conductivity measurements and Potentiometry.

Outcome:

- The scope of the subject is providing experimental facts and the principles to understand the kinetics and mechanism of various reactions.
- The subject emphasizes on various aspects of polarimetry studies including kinetic studies and comparing relative strength of acids.
- To acquire knowledge in qualitative and quantitative estimation of pure organic liquids and oils by using refractometry.
- To acquire knowledge to determine the viscosity of different mixtures
- To know how titrations can be done based on conductometric and potentiometric principles.
- To acquire knowledge in the principles regarding various equations and to determine the properties like solubility of sparingly soluble salts, pka values and the degree of ionization etc.,