

GURU NANAK COLLEGE (AUTONOMOUS)

(Affiliated to University of Madras and Re-Accredited at 'A' Grade by NAAC)

Guru Nanak Salai, Velachery, Chennai – 600042.



M.Sc. Chemistry

(SEMESTER PATTERN WITH CHOICE BASED CREDIT SYSTEM)

Syllabus

(For the candidates admitted in the Academic year 2019-20 and thereafter)

Vision

- ▣ To enhance the quality of education beyond the text book / syllabi based – exam oriented system to research and analytical based learning.
- ▣ To produce quality graduates and post graduates to excel in the field of education / research / industry.
- ▣ To encourage the learners of exceptional quality to take up research and motivate them to contribute to the needs of the society.
- ▣ To encourage the faculty to constantly involve themselves in research in addition to the regular work, which would enable them to develop research oriented learning skills.

Mission

- ▣ To inculcate the scientific methodology of learning chemistry by focusing more on practicals.
- ▣ To enhance the creativity in learning chemistry among the learners using visual aids.
- ▣ To produce and to modernize the infra structure to impart and understand the importance of practical skill accuracy and data interpretation.
- ▣ To encourage the learners to participate in the teaching – learning process to enhance their analytical and problem solving skill and to develop leadership qualities.
- ▣ To motivate the students by conducting seminars/workshops with the inputs of eminent scientists, distinguished alumni and industrialist.
- ▣ Visit to Industries and scientific centres to have exposure on sophisticated instruments and recent developments in chemistry.

PROGRAMME OUTCOME

At the completion of M. Sc. in Chemistry the students are able to:

PO 1: acquire a broad learning in advances in chemistry that stresses scientific reasoning and analytical problem solving with a molecular perspective and develop the ability to communicate scientific information in written and oral formats

PO 2 : expose broader experimentation in chemistry on applied aspect and also using modern instrumentation to understand the importance of the chemical transformation for high throughput applications.

PO 3: Investigate the interdisciplinary nature of chemistry in biology, medicine, materials science to excel in R&D for the benefit of societal needs. Have extra acquaintance in humanities other than chemistry.

PO 4: execute the laboratory skills needed to design, and interpret chemical research; acquire a foundation of research in chemistry

PO 5: develop the skills required to succeed in higher learning in chemistry, in the chemical industry and in academic profession.

PROGRAMME SPECIFIC OUTCOME

The students at the time of graduation will be able to

PSO 1: adopt to the major scientific and technological challenges in research, industry as they are well trained in experimental techniques like synthesis, separation, distillation, crystallization *etc.*

PSO 2 : compete in the international, National, state level assessments.

M.Sc (Chemistry)
COURSE STRUCTURE (2019-21) Batch

Semester	Course Component	Subject Code	Subject Name	Credits	Hours	CIA	ESE	Total
Semester – I	Core-1	19PCHE301	Stereochemistry and Reaction Mechanism	4	5	50	50	100
	Core-2	19PCHE302	Chemical Kinetics	4	4	50	50	100
	Core-3	19PCHE303	Coordination Chemistry	4	4	50	50	100
	Core-4	19PCHE304	Analytical Chemistry	4	4	50	50	100
	Core Practical-1	19PCHE305P	Organic Chemistry Practical-1	*	5	*	*	*
	Core Practical-2	19PCHE306P	Inorganic Chemistry Practical-1	*	4	*	*	*
	Core Practical-3	19PCHE307P	Physical Chemistry Practical-1	*	4	*	*	*
	Soft Skill - 1	19PGSL401	Personality Enrichment	2		50	50	100
Total Credits: 18 / Total Hours per week: 30								
Semester – II	Core-5	19PCHE308	Quantum chemistry and Group Theory	4	5	50	50	100
	Core-6	19PCHE309	Organometallics and Bioinorganic chemistry	4	4	50	50	100
	Core-7	19PCHE310	Chemistry of Aromatic compounds and Concerted reactions	4	4	50	50	100
	Core Practical-1	19PCHE305P	Organic Chemistry Practical-1	4	5	50	50	100
	Core Practical -2	19PCHE306P	Inorganic Chemistry Practical-1	4	4	50	50	100
	Core Practical-3	19PCHE307P	Physical Chemistry Practical -1	4	4	50	50	100
	Elective-1	19PCHE311	Chemistry of Natural Products	3	4	50	50	100
	Soft Skill - 2	19PGSL402	Computing Skill	2		50	50	100
Total Credits: 29 / Total Hours per week: 30								

Semester	Course Component	Subject Code	Subject Name	Credits	Hours	CIA	ESE	Total
Semester – III	Core-8	19PCHE312	Spectroscopy-1	4	5	50	50	100
	Core-9	19PCHE313	Synthetic Methodology	4	5	50	50	100
	Core-10	19PCHE314	Thermodynamics and Electrochemistry	4	5	50	50	100
	Core Practical-4	19PCHE315P	Electroanalytical Practical	*	5	*	*	*
	Elective Practical-1	19PCHE316P	Analytical Chemistry Practical	*	5	*	*	*
	Elective-II	19PCHE317	Solid state and Nano Chemistry	3	5	50	50	100
	Soft Skill-3	19PGSL403	Self and Time Management Skills	2	-	50	50	100
	Summer Internship **	19PINT401	Summer Internship **	2	-	50	50	100
Total Credits: 19 / Total Hours per week: 30								
Semester – IV	Core-11	19PCHE318	Photochemistry	4	5	50	50	100
	Core-12	19PCHE319	Spectroscopy-II	4	5	50	50	100
	Core Practical-4	19PCHE315P	Electroanalytical Practical	4	5	50	50	100
	Elective Practical-1	19PCHE316P	Analytical Chemistry Practical	4	5	50	50	100
	Soft skill-4	19PGSL404	Spoken and Presentation Skills	2	-	50	50	100
		19PCHE320	Group project	6	10	50	50	100
	Total Credits: 24 / Total Hours per week: 30							
Grand Total Credits: 90 / Total Hours per week: 120								

* Practical Examinations are conducted once in an Academic year - at the end of semester II and semester IV.

** The students should undergo summer internship for three weeks after the second semester and the reports to be submitted

SEMESTER - I

GURU NANAK COLLEGE (AUTONOMOUS), CHENNAI – 600042

(Effective for the batch of candidates admitted in 2016–17)

**CORE-I
STEREO CHEMISTRY AND REACTION MECHANISM**

SUBJECT CODE: 19PCHE301	THEORY	MARKS :100
SEMESTER:I	CREDITS:4	TOTAL HOURS : 60

COURSE OBJECTIVES:

- This course aims to explain basic concepts in stereo chemistry and methods of determining reaction mechanisms.
- To explain synthetic application of aliphatic nucleophilic substitution, elimination reactions in organic synthesis.

UNIT-I: Stereochemistry-I (15 hrs)

Optical activity - chirality- conditions for optical activity-asymmetry and dissymmetry-dissymmetry of allenes, biphenyls, para cyclophanes, ansa compounds and molecules with helical structures - absolute configuration- D/L and R/S notation of acyclic chiral molecules, allenes, biphenyls and spiro compounds-molecules with more than one asymmetric centre - erythro/threo and meso/dl configuration - Fischer Projection-Newmann and Saw horse projection-inter conversion of projection formulae- prochiral centre- - Cram's rule and Prelog's rule - optical purity – enantiomeric excess–stereo specific and stereo selective reactions.

Geometrical isomerism: E-Z nomenclature of olefins and oximes - Geometrical and optical isomerism of mono and disubstituted cyclopropane, cyclobutane, cyclo pentane and cyclo hexane derivatives - homotopic, enantiotopic and diastereotopic hydrogen - prochiral carbon (up to 10 carbons only)-pro R and pro S &Re and Si face-determination of configuration.

UNIT-II: Stereochemistry-II (10 hrs)

Conformation and conformational analysis - conformation of simple 1,2- di-substituted ethane derivatives-cyclo propane, cyclobutane, cyclo pentane and cyclohexane derivatives - conformational free energy –

conformation analysis of mono and di-substituted cyclohexanes and their stereo chemical feature (geometrical and optical isomerism)-conformation and stereo chemistry of decalin and 9 -methyl decalin-conformation of glucose.

Conformation and reactivity: steric and product development control– reduction of tertiary butyl cyclo hexanone by hydride –stereo chemistry of oxidation of cis and trans tertiary butyl cyclo hexanols by Cr (VI) – stereochemistry of the reaction between nitrous acid and α -amino cyclo hexanols. Asymmetric synthesis: Evans and Enders

UNIT-III : Methods of Determining Reaction Mechanisms (15hrs)

Kinetic and non-kinetic methods of determining reaction mechanisms- Thermodynamic and kinetic aspects - spectroscopic studies – Hammond's postulate - isotope effects – energy profile diagrams – intermediate vs transition state – product analysis and its importance – cross over experiments.

Quantitative treatment of structure and reactivity – Hammett and Taft equations Classification of solvents, solvent effects in organic chemistry – solute – solvent interactions –specific and non-specific selective solvation.

S_N1 , S_N2 and S_{Ni} mechanism – neighbouring group participation – reactivity, structural and solvent effects – substitution in norbornyl and bridgehead systems– substitution by ambident nucleophiles such as cyano, nitro, phenoxide and ambident dianions – substitution at carbon doubly bonded to oxygen and nitrogen – alkylation and acylation of amines, halogen exchange, Von-Braun reaction, alkylation and acylation of active methylene carbon compounds, hydrolysis of esters, Claisen and Dieckmann condensations.

UNIT - IV: Organic Reaction Mechanisms - Addition to carbon-carbon and carbon-hetero multiple bonds (10hrs)

Mechanism - Electrophilic, nucleophilic and free radical addition. Addition of halogen, nitrosyl chloride to olefins, Hydration of olefins and acetylenes. Hydroboration, Hydroxylations and Michael addition. Diels-Alder reaction, 1,3 -dipolar additions. Carbene and their addition to double bonds- Simmon Smith reaction, Mannich, Stobbe, Darzen, Wittig, Wittig-Horner and Benzoin reactions. Nitrene: Methods for generating nitrenes and their reactions. (Stereo chemical aspects to be studied wherever applicable).

UNIT–V: Elimination Reactions (10 hrs)

E_1 , E_2 and E_1CB mechanism – spectrum, orientation of the double bond - Hoffman and Saytzeff rule – competition, elimination and substitution. Typical eliminations to be studied –dehydration, dehydro-halogenation and similar reactions. Stereochemistry of E_2 eliminations in cyclohexanes and bicyclic systems. Mechanism of pyrolytic elimination. Examples : Chugaev and Cope elimination.

TEXTBOOKS:

1. E. Eliel, S.H. Wilen and L.N. Mander, Stereochemistry of Carbon Compounds, John Wiley & Sons, New York, second edition, 1994.
2. D. Nasipuri, Stereochemistry of Organic Compounds, Wiley Eastern Ltd, New Delhi, second Edition, 1994.
3. P.S. Kalsi, Stereochemistry, Conformation and Mechanism, New Age International Ltd, sixth edition, 2006.
4. P.S. Kalsi, Stereochemistry and Mechanism Through Solved Problems, New Age International Ltd, third edition, 2001.
5. J. March, Advanced Organic Chemistry; Reactions, Mechanisms and Structure, Wiley inter science, sixth edition, 2007.
6. R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Organic chemistry, Pearson Prentice hall, seventh edition, 2012.
7. P.S. Kalsi, Organic reactions and their Mechanism, New Age International Ltd, third edition, 2012.

REFERENCEBOOKS:

1. K.Mackie, M.Smith, P.Aitken, Guide Book to Organic Synthesis, ELBS, England, third edition, 2000.
2. R. Bruckner, Advanced Organic Chemistry Reaction Mechanism, Elsevier, New Delhi, 2002.
3. T.L.Gilchrist and C.W.Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London, 1967.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, second edition, 2014.
5. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Parts A and B .Springer, fifth edition, 2015.

Question paper pattern:

Section	Question Component	Numbers	Marks	Total
Section A	MCQ:1-10 , Fill up : 11-15 , T/F:16-20 Answer all questions	1 – 20	1	20
Section B	Short Answer / Problems Answer any 5 out of 8 questions	21–28	7	35
Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTALMARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit– 1	4	
	Unit– 2	4	
	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	1	1
	Unit– 2	1	
	Unit– 3	1	1
	Unit– 4	1	
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

CORE-2
CHEMICAL KINETICS

SUBJECT CODE: 19PCHE302	THEORY	MARKS : 100
SEMESTER : I	CREDITS : 4	TOTAL HOURS : 60

COURSE OBJECTIVES:

- To learn the basic concepts in chemical kinetics, enzyme kinetics, surface reactions and fast reactions.

UNIT- I (15 hrs)

Effect of temperature on reaction rates-collision theory of reaction rates-molecular beams-collision cross sections-effectiveness of collisions -probability factors-potential energy surfaces-partition functions-and activated complex. Eyring equation-estimation of free energy and entropy of activation and their significance.

UNIT-II (10 hrs)

Reactions in solutions- effect of pressure, dielectric constant and ionic strength on reactions in solutions-kinetic isotope effects-linear free energy relationships-Hammett and Taft equations.

UNIT- III (10 hrs)

Acid base catalysis-mechanism of acid base catalyzed reactions-Bronsted catalysis law. Catalysis by enzymes-rate of enzyme catalyzed reactions-effect of substrate concentration, pH and temperature on enzyme catalyzed reactions- Inhibition of enzyme catalyzed reactions.

UNIT-IV (10 hrs)

Langmuir and BET adsorption isotherms-adsorption coefficient and its significance. Kinetics and mechanism of surface reactions-surface reactions catalyzed by metals, semiconductor oxides.

UNIT- V (15 hrs)

Kinetics of complex reactions - reversible reactions-consecutive reactions - parallel reactions - Chain reactions - general treatment of chain reactions - Rice - Herzfeld mechanism and explosion limits. Study of fast reactions - relaxation

methods - temperature and pressure jump methods-stopped flow and flash photolysis methods.

TEXT BOOKS:

1. J.Rajaram and, J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations, McMillan India Ltd., third edition, reprint, 2009.
2. K.J.Laidler, Chemical Kinetics. Harper and Row, Pearson Pvt.Ltd, New York, third edition, 2011.
3. K.L. Kapoor, A textbook of Physical Chemistry, Macmillan India Ltd, reprint, 2010.

REFERENCE BOOKS:

1. W.J. Moore, Physical Chemistry, Orient Longman, London, fourth edition,1963.
2. G.M. Barrow, Physical Chemistry, Tata McGraw Hill, fifth edition,2008.
3. R.G. Frost and Pearson, Kinetics and Mechanism, Wiley, New York ,third edition, 1981.
4. W.J. Moore and R.G. Pearson, Kinetics and Mechanism, Wiley New York, third edition, 1981.
5. I. Amdur and G.G. Hammes, Chemical Kinetics, Principles and selected topics, McGraw Hill, New York, 1968.
6. G.M. Harrus, Chemical Kinetics, D.C. Health and Co., 1966.

Question paper pattern:

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Section A	MCQ:1-10 , Fill up : 11-15 , T/F:16-20 Answer all questions	1 – 20	1	20
Section B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTALMARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit- 1	4	
	Unit- 2	4	
	Unit- 3	4	
	Unit- 4	4	
	Unit- 5	4	
Section B	Unit- 1	1	1
	Unit- 2	1	
	Unit- 3	2	
	Unit- 4	1	
	Unit- 5	2	
Section C	Unit- 1	1	
	Unit- 2	1	
	Unit- 3	1	
	Unit- 4	1	
	Unit-5	1	

CORE THEORY– 3
COORDINATION CHEMISTRY

SUBJECT CODE:19PCHE303	THEORY	MARKS - 100
SEMESTER : I	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To impart the theories about bonding structure and important properties of various coordination complexes.

UNIT-I: Bonding and Properties of complexes (15 hrs)

Crystal Field Theory (CFT) - crystal field effects in tetrahedral, octahedral & square-planar symmetries, CFSE, spectro chemical series and applications. High spin and low spin complexes-Magnetic properties of coordination compounds. Nephelauxetic effect, Molecular orbital theory-Based on group theoretical approach, Symmetry of molecular orbitals formed from atomic orbital overlap, LCAO-MO model, TASO, LUMO and HOMO concepts in bonding. M.O.diagrams of octahedral, tetrahedral and square planar complexes. Calculation of Δ_o and Δ_t and their relationship, Jahn-Teller tetrahedral distortion.

Unit-II: Stability and Stereoisomerism of Coordination Complexes (10 hrs)

Stability of complexes-Thermodynamic stability-stepwise and overall stability constants and their relationships. Factors affecting the stability of the complexes, HSAB approach, Chelate effect, importance of chelates. Determination of stability constants by spectrophotometric, polarographic and potentiometric methods. Stereoisomerism in inorganic complexes, Optical rotatory dispersion (ORD) and circular dichroism (CD), Stereochemical aspects of substitution reaction of Octahedral Complexes, Stereochemical changes in dissociation (S_N2) and displacement (S_N2) mechanism through various geometries of coordination compounds. Isomerization and racemization reactions in octahedral complexes.

UNIT-III:Coordination Chemistry-Reaction Mechanisms (15 hrs)

Electron transfer reactions; outer and inner sphere processes; atoms transfer reactions. Key ideas concerning electron transfer between transition metals. Chemical activation and electron transfer, mechanism of electron transfer reactions-nature of the bridging ligand and its role in rate of reaction. Two electron transfer reactions and non-complementary reactions. Cross reactions and thermodynamics-Marcus-Hush theory

and equation.

UNIT-IV: Substitution Reactions in Coordination compounds (10 hrs)

Substitution reactions in square planar complexes - the rate law - influences of entering, leaving and other groups, the trans effect - theories - mechanism of nucleophilic substitution in square planar complexes and octahedral complexes (cobalt and chromium) - replacement of coordinated water, solvolytic (acids and bases) reactions, applications in synthesis (platinum and cobalt complexes only). Kinetics of octahedral substitution - ligand fields effects and reaction rates. Rearrangement in 4 and 6 coordinate complexes: reaction at coordinated ligands-template effect.

UNIT-V: Coordination Chemistry of Special Compounds (10 hrs)

Clusters: Boranes, carboranes, metallo boranes and metallo carboranes-synthesis and structure of neutral boron hydrides, polyhedral borane anions and dianions, Capping rules, PSEPT (Wade's rules). Low nuclearity metal-carbonyl clusters and $14n+2$ rule, high nuclearity metal-carbonyl clusters with internal atoms. Isopoly and heteropoly acids and salts (Mo, W, V, Nb and Ta), Heteropoly anions-structure and reactivity; heteropoly blues.

Boron-nitrogen compounds: azaboranes, pyrazaboles, borazines and B-N clusters. P-N and P-S compounds : poly phosphazene and cyclic amino phosphanes, phosphorus-oxide and phosphorus-sulfide cages. Sulfur-nitrogen compounds. Macrocyclic ligands; types- Schiff bases; crown ethers and cryptands.

TEXT BOOKS:

1. J.E.Huheey, Inorganic Chemistry-Principles, Structure and Reactivity; Harper Collins, NY, fourth edition, 1993.
2. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry-A Comprehensive Text ,John Wiley & Sons, fifth edition, 1988.
3. K.F.Purcell and J.C.Kotz, Inorganic Chemistry, Sengage Learning India Pvt. Ltd, first edition, 2010.
4. M.C.Dayand J.Selbin, Theoretical Inorganic Chemistry, Literary Licensing, LLC, 2012.
5. A.E.Martell, Coordination Chemistry, Vol. I, Van Nostrand-Reinhold, 1971.

REFERENCE BOOKS:

1. R.L.Carlin, Transitionmetal Chemistry, Vol.1to 5,Academic Press,London,1968..F.Shriver,P.W.Atkins and C.H.Langford, Inorganic Chemistry, Oxford Univ. press, NewYork, secondedition.1994.

- I. G. Wilkinson, Comprehensive coordination Chemistry, Vol.1, Elsevier, 1987.
- F. Basolo and R. G. Pearson, Inorganic reaction mechanism, John Wiley, New York, second edition, 1967.
- R. A. Henderson, Mechanisms of Reactions at transition metal sites, Oxford Scientific. Publication, 1995.

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Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTAL MARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit– 1	4	
	Unit– 2	4	
	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	2	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	2	
	Unit– 5	2	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit– 5	1	

CORE THEORY– 4
ANALYTICAL CHEMISTRY

SUBJECT CODE: 19PCHE304	THEORY	MARKS -100
SEMESTER:I	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To create the better understanding of “Analytical Chemistry”; to evolve proper analytical data and practice to report the result with uncertainty.
- To initiate the better understanding in the analysis of complex materials and also the finished products of chemical manufacturing units.
- To introduce the instrumental based chemical analysis in all the arena of chemical processes.
- To establish the competency of chemical analysis in the applied research, chemical processes and testing/quality control laboratories.
- To eliminate the gap between academic and industry and also the basic and applied science.

UNIT - I: Fundamentals in Chemical Analysis and Analytical Laboratory Functioning (10hrs)

Concepts and perspectives of analytical chemistry; Errors and treatment of analytical data :Accuracy, Precision, Errors and types, minimization of errors, significant figures, mean, median, regression analysis - Standard deviation - Comparison of results- F, T and Q tests. Calibrations –General idea of calibration, calibration of glasswares, balance, instruments and other equipment. Uncertainty in chemical analysis: theory, significance, sources of uncertainty for simple volumetric analysis.

Details on method development and method validation in chemical analysis, essentials of quality control and quality assurance systems in chemical processes; Basic idea and necessity of accreditations / certification such as GLP, ISO (NABL) and FDA. Role of ISI and Agmark on the consumer products.

UNIT-II: Instrumental Methods of Analysis and Analysis of Complex Materials (15hrs)

Theory, instrumentation and applications of Atomic absorption spectroscopy, ICP-MS; Flame emission spectrometry and ICP-OES. Application of these techniques in water and food analysis. Moisture analyzer (KFR method)and C,H, N analysis (instrumental methods).

Sampling of solid, liquid and gases–primary sample, laboratory sample, analytical

sample, handling, collection, transport, storage. Physico-chemical analysis of medicines (formulated), ores, fertilizers, alloys, packed foods, water and air. [Note: Any one representative example in each category and testing of important parameters only]

UNIT-III: Separation Techniques (15hrs)

Chromatographic techniques : General aspects ,classification, principle, instrumentation (if applicable) and applications of column, ion-exchange, electrophoresis, TLC, paper chromatography, GLC and HPLC (with different detectors) and GPC. Special emphasis on GC-MS, GC-MS / MS, LC-MS,LC-MS / MS. Role of chromatographic techniques in R&D and quality control laboratories.

UNIT-IV: Electro analytical Methods (12hrs)

Polarography – Theory, Instrumentation, type of currents (includes kinetic & catalytic currents), advantages of DME. Ilkovic equation (No derivation) and its significance. Qualitative and quantitative applications to the analysis of inorganic compounds and determination of dissolved oxygen. Derivative Polarography – Amperometry and bi amperometry (theory, equipment and applications). Cyclic voltammetry – theory, instrumentation and applications to inorganic and organic compound. Application of CV in applied research viz., prediction of reaction mechanism, redox behavior of chemical compounds and identification of number of electrons in the electro chemical processes.

UNIT-V: Thermal, Radio-analytical Methods (8 hrs)

Principle, instrumentation and applications of TGA, DTA and DSC. Radio analytical methods - Principle, instrumentation and applications of neutron activation and isotopic dilution analysis. Radiometric titrations, determination of age of fossils, radiometric methods in diagnosis o f diseases.

TEXTBOOKS:

1. David Harvey; Modern Analytical Chemistry; McGraw-Hill, first edition, 2000.
2. J.Mendham, R.C.Denney, J.D.Barnes and M.Thomas, Vogel's Textbook of quantitative Chemical Analysis; Pearson Education Pvt.Ltd. sixth edition, 2004.

REFERENCEBOOKS

1. E Prichard, Quality in the analytical chemistry laboratory, John Wiley and sons, 1997.
2. W. Funk, V Dammann, G. Donne vert, Quality assurance in analytical, VCH Weinheim, 1995.
3. Douglas A. Skoog, Donald M. West and F. James Holler, Fundamentals of Analytical Chemistry; ninth edition, Harcourt AsiaPvt.,Ltd.,2001.
4. Douglas A. Skoog, Donald M. West and F. James Holler, Analytical Chemistry: An Introduction; seventh edition, Saunders College Publishers, 2000.
5. Dean, John A. Merritt, LynneL. , Jr.Settle, Frank A., Jr.Willard, Hobart H; Instrumental Methods of Analysis, Wadsworth Publishing, seventh Edition, 1988.
6. D.A. Skoog, Principles of Instrumental Analysis, 5th ed., Saunders College Publishing, Philadelphia, London, 1998.
7. A.J. Bard and L.R. Faulkner, Electrochemical Methods,JohnWiley,1980.
8. S.M. Khopkar, Environmental Pollution Analysis, New Age International publication, 2011.
9. Seonard 'l Ciacere, Water and water pollution (handbook), Vol I to IV, Marcel Dekkerinc.N.Y.1972.
10. Guidelines for drinking-water quality, third edition, (incorporating first and second addenda),WHO report.
11. Martin Hocking, Handbook of chemical technology and pollution control, AP Publication, third edition, 2005.
12. Chemical analysis of metals; Sampling and analysis of metal bearing ores: American Society for Testing and Materials Technology& Engineering, 1980.
13. Manual of Procedures for Chemical and Instrumental Analysis of Ores, Minerals, and Ore Dressing Products. Government of India Ministry of Steel & Mines, Indian Bureau of Mines,1979.
14. Yeshajahu Pomeranz, Clifton E. Meloan, Food Analysis: Theory and practice, Springer, third edition, 2002.
15. George Charalanbous, Analysis of food and beverages, Academic press,1978.
16. Connor's Text book of Pharmaceuticals Analysis, John-wiley, third edition, 2001.
17. Encyclopaedia of industrial chemical analysis, Snell et al; Interscience,1966.

Visits to:

- i. GLP, ISO & FDA certified R&D and QC laboratories.
- ii. Various chemical industries with established laboratories.
- iii. BIS & FSSAI approved establishments.

Question paper pattern:

Section	Question Component	Numbers	Marks	Total
Section A	MCQ:1-10 , Fil lup : 11-15 , T/F: 16-20 Answer all questions	1 – 20	1	20
Section B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTAL MARKS				100

Distribution of Questions;

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit– 1	4	
	Unit– 2	4	
	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	1	1
	Unit– 2	1	
	Unit– 3	1	1
	Unit– 4	2	
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

SEMESTER - II

CORE THEORY –5
QUANTUM CHEMISTRY AND GROUP THEORY

SUBJECT CODE :19PCHE308	THEORY	MARKS:100
SEMESTER:II	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To learn the basic concepts in group theory and the need for quantum mechanics and appreciate their significance.

UNIT-I : Quantum Chemistry–I (10 hrs)

Inadequacy of classical theory - black body radiation - photo electric effect- Compton effect-Bohr's Quantum theory and subsequent developments-wave particle duality-de Broglie equation-Heisenberg's uncertainty principle.

Quantum mechanical postulates - The Schrodinger equation- elementary applications of Schrodinger equation- the particle in a box (one, two and three dimensional cases) – particle in a ring.

UNIT-II: Quantum Chemistry–II (10 hrs)

The harmonic oscillator- the rigid rotor-the hydrogen atom-the Schrodinger equation for hydrogen atom – the solution – the origin of quantum numbers (angular momentum and spin) - their physical significance.

UNIT–III: Quantum Chemistry – III (15 hrs)

Approximation methods – perturbation and variation method- Application to hydrogen, helium atoms-R-S coupling, j-j coupling and term symbols for atom in ground state - Slater rules, Slater orbital and HFSCF methods - Born-Oppenheimer approximation-Valence Bond theory for hydrogen molecule–LCAO–MO theory for di and polyatomic orbitals-concepts of hybridization- Huckel theory for conjugated molecules (ethylene, butadiene and benzene) semi empirical methods.

UNIT–IV: Group Theory-I (10 hrs)

Symmetry elements and symmetry operations - point groups-identification and determination. Reducible and irreducible representations-direct product representation - Orthogonality theorem-its consequences-character table

UNIT– V:Grouptheory–II (15 hrs)

Hybrid orbitals in non-linear molecules-(CH₄, XeF₄, BF₃, SF₆ and NH₃). Symmetry based selection rules for infrared, Raman and electronic spectra of ethylene and formaldehyde-application of group theory.

TEXTBOOKS:

1. D.A. McQuarrie, Quantum Chemistry, University Science books, viva books Pvt. Ltd, second edition, reprint, 2007.
2. I.N. Levine, Quantum Chemistry, Pearson Education Pvt.Ltd, fifth edition,2004.
3. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India Limited, first edition, 2000.
4. R.K. Prasad, Quantum Chemistry, New Age India, fourth edition,2010.
5. V. Ramakrishnan and M.S. Gopinathan, Group theory in Chemistry, Vishal publications.1 988.
6. K.V. Raman, Group theory and its applications in Chemistry, Tata McGraw Hill,1990.
7. S.Swarnakakshmi, T.Saroja, R.M.Ezhilarasi, A Simple approach to group theory in Chemistry, Universities Press, first edition 2008.
8. R.K.Prasad Quantum Chemistry-theory solved problems and solutions, New Age International Pvt. Ltd, 2009.

REFERENCEBOOKS:

1. F.A. Cotton, Chemical application of group theory, John Wiley & Sons Inc., New Delhi, third edition, 2009.
2. Alan Vincent, Molecular Symmetry and Group theory-Programmed introduction to chemical applications, Wiley, New Delhi, 2010.
3. H. Eyring ,J. Walter and G.Gimball, Quantum Chemistry, John Wiley & Sons Inc.,NewYork,1944.
4. L.S. Pauling and F.B. Wilson, Introduction to quantum mechanics, McGraw Hill Book Company, New York, 1935.
5. P.W. Atkins, Molecular quantum mechanics, Oxford University Press, Oxford, third edition,1997.
6. David, J. Griffiths, Introduction to Quantum mechanics, dorling kinderly Pvt. Ltd, second edition, fifth reprint, 2008.

Question paper pattern:

Section	QuestionComponent	Numbers	Marks	Total
Section A	MCQ:1-10 , Fill up : 11-15 , T/F:16-20 Answer all questions	1 – 20	1	20
Section B	Short Answer /Problems Answer any 5 out of 8 questions	21–28	7	35
Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTAL MARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit– 1	4	
	Unit– 2	4	
	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	1	1
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	1
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

CORETHEORY-6
ORGANO METALLICS AND BIOINORGANIC CHEMISTRY

SUBJECT CODE: 19PCHE309	THEORY	MARKS :100
SEMESTER:II	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- This paper exposes the student to the basics of organo metallic Chemistry, Reactions of organo metallic complexes and their Industrial applications.

UNIT-I: Introduction to Organometallics (15hrs)

Valence electron count and 16/18 electron rules for organometallic compounds; structure and bonding in mono and polynuclear metal carbonyls; backbonding and synergic effect- π -acids, vibrational spectra of metal carbonyls; dinitrogenas ligand in organometallic compounds. Synthesis, structure and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes;

UNIT-II: Reactions of organometallic complexes (10hrs)

Synthesis, structure and bonding of metallocenes and bent metallocenes; organo metallic reactions: association, substitution, addition, oxidative addition, reductive elimination, insertion and deinsertion, electrophilic and nucleophilic attack on ligand sand fluxional isomerism.

UNIT-III: Industrial Application of Organometallic Compounds (8hrs)

Catalytic applications of organo metallics: Hydrogenation of olefins, Wacker-Smidt synthesis, oxo process, Repp's catalyst, Monsanto acetic acid process, Zeigler- Natta polymerization of alkenes and oligomerisation, Enantio selective functional group interconversions. Trans metallation and cyclization reaction of organo metallics. Bio organo metallic chemistry and surface organo metallic chemistry.

UNIT-IV: Introduction of Bio-inorganic chemistry (15hrs)

General properties of biological molecules. Physical methods in bio-inorganic chemistry. Metal Storage, Transport and Biomineralisation; Ferritin, Transferrin and siderophores, sodium and potassium ion balance. Essential and trace metal ions. Metallo enzymes-Zinc enzymes- carboxy peptidase and carbonic

anhydrase, Vitamin B₁₂, catalase, peroxidase, superoxide dismutase and copper proteins. Application of Coordination compounds in medicinal applications.

– Cisplatin – anti rheumatoid - gold compound –anti diabetic - anti cancer agents – role of metal ion diagnosis and treatment.

UNIT–V: Transport Proteins (12hrs)

Oxygen Carriers – Haemoglobin, myoglobin – structure – function - Oxygenation and stereochemistry – Bohr effect, Non – heme oxygen carriers – Hemerythrin and Haemocyanin. Biological redox systems: cytochromes – classification, cytochrome a, b and c. Cytochrome P-450, Iron – sulphur proteins – rubredoxin and ferridoxin. Chlorophylls and photosynthesis –structure, function and mechanism. Nitrogen fixation – introduction – types of nitrogen fixing micro organisms, Nitrogen as eenzyme–Metal clusters in nitrogenase –redox property– Dinitrogen complexes–nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia.

TEXT BOOKS:

1. Ram C. Mehrotra and A.Singh, Organometallic Chemistry, A Unified Approach, New Age International, second edition, 2004.
2. B.D.Gupta and A.J.Ellas, Basic Organometallic Chemistry, Concepts, Syntheses and Applications, Universities press, 2010.
3. K.Hussain Reddy, Bioinorganic chemistry, New Age International private Ltd, reprint 2005.
4. William W. Porterfield, Inorganic Chemistry, An unified approach, academic press inc, 1993.

REFERENCEBOOKS:

1. G.N. Mukherjee and Arabinda Das, Elements of Bioinorganic Chemistry, U. N. Dhar & Sons Pvt .Ltd., Kolkata [ISBN 81-85624-37-2].
2. M.Satake and Y.Mido, Bioinorganic Chemistry, Discovery Publishing House, New Delhi, 2011.
3. Asim K. Das – Bioinorganic Chemistry, Books & Allied (p) Ltd, first edition, 2004.

Question paper pattern:

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	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	2	
	Unit– 2	2	
	Unit– 3	2	
	Unit– 4	1	
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

CORE THEORY – 7
CHEMISTRY OF AROMATIC COMPOUNDS AND CONCERTED REACTIONS

SUBJECT CODE:19PCHE310	THEORY	MARKS:100
SEMESTER:II	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- This paper explains the concepts of aromatic compounds, their electrophilic and nucleophilic substitution reactions. In addition, mechanism of some of the important rearrangements and pericyclic reactions in organic chemistry will be discussed. The first part of the course brings forth the salient features of oxidation and reduction reactions in organic synthesis.

UNIT-I: Oxidation and Reduction (15 hrs)

Mechanism – study of the following oxidation reactions – use of chromium(VI), MnO_4^- , MnO_2 , TPAP, Moffatt, Oppenauer and Swern oxidation of alcohol–oxidative cleavage of glycols and their related compounds, Oxidative cleavage of ketones, aldehydes and acohols, Ozonolysis -oxidation of methylene to carbonyl, oxidation of aryl methane – allylic oxidation of olefins.Reductions:catalytic hydrogenation–Hydrides–Nucleophilic and Electrophilic-MPV reduction-Selectivity in reduction of 4-t-butyl cyclo hexanone susings electrides-Synthetic importance of Clemmensen and Wolf-Kishner reductions-Modifications of Wolf-Kishner reduction-Birch reduction.

UNIT–II:Aromaticity(10 hrs)

Concept of aromaticity, Huckel’s rule, Craig’s rule – Huckel MO theory of aromaticity –frost cycle - Alternant and Non-alternant hydrocarbons –Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds –systems with 2, 4, 8 and 10 electrons – Annulenes (up to C18) -Concept of homo aromaticity– Hetero aromatic molecules.

UNIT–III:AromaticElectrophilic,Nucleophilicsubstitution(15 hrs)

The arenium ion mechanism. Orientation and reactivity of mono nuclear, poly nuclear aromatic hydrocarbons (Naphthalene, Anthracene) and Heterocyclic

compounds (Quinoline and Isoquinoline) nitration, halogenations, sulphonation, alkylation, acylation and diazonium coupling. Formylation reactions (Gattermann, Gattermann-Koch, Vilsmeier-Haack and Riemer-Tiemann Reaction)- Synthesis of di and tri substituted benzenes (symmetrical tri bromo benzene, 2-Amino-5-methylphenol, 3-nitro-4-bromobenzoic acid, 3,4-dibromo nitrobenzene, 1,2,3-trimethylbenzene) starting from benzene or any mono substituted benzene.

Aromatic nucleophilic substitution: Methods for the generation of benzyne intermediate and reactions of aryl intermediate- Nucleophilic substitution involving diazonium ions. Aromatic nucleophilic substitution of activated halides. Ziegler alkylation. Chichibabin reaction and Von-Richter rearrangement.

UNIT-IV: Molecular Rearrangements (10 hrs)

Rearrangement to electron deficient carbon- Pinacol-Pinacolone, Wagner-Meerwein rearrangement, Benzil-Benzilic acid rearrangement, Arndt-Eistert synthesis. Rearrangement to electron deficient nitrogen-Hoffman, Curtius, Schmidt, Lossen, Beckmann Rearrangement to electron deficient oxygen- Baeyer-Villiger, Dakin reaction. Rearrangement to electron rich carbon- Favorski, Wittig, Neber, Stevens, Sommelet-Hauser.

UNIT-V: Pericyclic Reactions (10 hrs)

Introduction-Construction of π molecular orbitals of ethylene and 1,3-Butadiene, Symmetry in π molecular orbitals - Classification-Electrocyclic reactions-Woodward Hoffmann rule- $(4n + 2)\pi$ and $(4n)\pi$ systems- Ring opening and ring closing reactions - Interconversion of cyclobutene-butadiene system and interconversion of cyclohexadiene-hexatriene, FMO analysis, Correlation diagram method.

Cyclo addition- Woodward Hoffmann rule in $(\pi 2s + \pi 2s)$ and $(\pi 4s + \pi 2s)$ cyclo addition reactions - FMO analysis and Correlation diagram method. Diels-Alder reaction- Retro Diels-Alder reactions. Cheletropic Reactions-[2+2] Cheletropic cyclo addition, Cheletropic Elimination (Basic idea only) Sigmatropic rearrangements - Classification- Woodward- Hoffmann rule - FMO analysis of [1,3], [1,5] and [1,7] hydrogen shift reactions-carbon shift reactions .[3,3] sigmatropic shifts -Cope and Claisen Rearrangement-Degenerate Cope reaction. Fluxional isomerism-semibullvalene and bullvalene.

TEXT BOOKS:

1. R.Bruckner, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi. 2002
2. J.March, Advanced Organic Chemistry, John Wiley & Sons Singapore, fourth edition,2009.
3. T.L.Gilchrist and C.W.Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London, 1967.
4. Niellissac, Physical Organic Chemistry, Prentice Hall, second edition,1996.
5. Jagdamba Singh and Jaya Singh, Photo chemistry and Pericyclic reaction, New Age International (P) Limited publisher, third edition, 2014.
6. P.S.Kalsi, Organic Reaction and Mechanism, NewAge International Pvt Ltd, third edition, 2012.

REFERENCE BOOKS:

1. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A and Part-B, Springer (INc), fifth edition, 2015.
2. J.Clayden, N.Greeves, S.Warren and P.Wothers, Organic Chemistry, Oxford University Press, second edition, 2014.
3. R.O.C.Norman and J.M.Coxon, Principles of organic synthesis, CRC Press, third edition, 2012.
4. W.Carruthers and Goldham, Some Modern Methods of Organic Synthesis, Cambridge University Press, fourth edition, 2012.
5. H.O.House, Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London,1972.

Question paper pattern:

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Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTAL MARKS				100

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	Unit- 2	4	
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	Unit- 4	4	
	Unit- 5	4	
Section B	Unit- 1	2	
	Unit- 2	1	
	Unit- 3	1	1
	Unit- 4	1	
	Unit- 5	1	1
Section C	Unit- 1	1	
	Unit- 2	1	
	Unit- 3	1	
	Unit- 4	1	
	Unit-5	1	

CORE PRACTICAL –1
ORGANIC CHEMISTRY PRACTICAL–I

SUBJECT CODE: 19PCHE305P	PRACTICAL	MARKS :100
SEMESTER:II	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- The practical is designed to give an exposure to lab techniques in analysis of organic molecules and synthesis of simple organic compounds.
- To provide the basic training for extraction of compounds from natural products and chromatographic separation.

I. Analysis of a mixture of the organic compounds.

Identification of components in a two component mixture and preparation of their derivatives. Determination of b.p./m.p. for components and m.p. for the derivatives.

II. Preparation of an organic compounds

a. Single stage (Any five)

1. Preparation of o-benzyl benzoic acid
2. p-Nitro benzoic acid from p-Nitro toluene
3. Anthro quinone from anthracene
4. Benzhydrol from benzophenone
5. m-Nitro aniline from m-dinitrobenzene
6. 1,2,3,4-Tetrahydrocarbozole from cyclohexanone
7. p-chlorotoluene from p-toluidine
8. 2,3-Dimethylindole from phenyl hydrazine and 2-butanone (boiling acetic acid)
9. Methyl orange from sulphanilic acid
10. Diphenyl methane from benzyl chloride

b. Two stage* (anythree):

1. Sym-Tribromobenzene from aniline.
2. p-nitroaniline from acetanilide
3. m-Nitrobenzoic acid from methyl benzoate.
4. 2,4-Dinitrobenzoic acid from p-nitrotoluene.
5. m-Nitrobenzoic acid from benzaldehyde
6. p-bromo aniline from acetanilide

IIIA) Extraction of natural products*(any two)

1. Caffeine from tea leaves

2. Lactose from milk
3. Citric acid from lemon
4. Piperine from black pepper

B) Chromatographic Separations:*

1. Column chromatography-separation of anthracene and acid from anthracene picrate.
2. Thin layer chromatography separation of green leaf pigments.
3. Paper chromatography
4. Identification of amino acids

C) Quantitative estimation of common drugs*

1. Estimation of vitamin C in tablets by Iodimetry.
2. Estimation of Aspirin by spectrophotometry

****Only for Internal Assessment***

RECOMMENDED BOOKS:

1. Brian S. Furniss, Antony J. Hannaford, Peter W.G. Smith, Austin R. Tatchell, Vogel's Text Book of Practical Organic Chemistry; Dorling Kindersley (India) Pvt. Ltd., fifth edition, 2011.
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, New Age Intl. Pvt. Ltd., fifth edition, reprint 2013.
3. Mann and Saunders, Laboratory manual of Organic Chemistry, Orient-Longman, fourth edition, 2004.

**CORE PRACTICAL –II
INORGANIC CHEMISTRY PRACTICAL-I**

SUBJECT CODE: 16PCHC06P	PRACTICAL	MARKS:100
SEMESTER:II	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To train the candidate in inorganic compound preparation, separation of the two metal ions by chromatographic method and deduction identification of cations by semi micro method.

EXPERIMENTS

a. Semi micro qualitative analysis: A mixture containing two common and two rare cations. The following are the rare cations to be included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, U and Li.

b. Complexometric titrations (EDTA) -Estimation of Ca, Mg and Zn.

c. Preparation of the following:

1. Potassium tris(oxalato)aluminate(III)trihydrate.
2. Tris(thiourea)copper(I) chloride
3. Potassium tris(oxalato)chromate(III) trihydrate
4. Sodium bis(thiosulphato)cuprate(I)
5. Tris(thiourea)copper(I) sulphate
6. Sodium hexanitrocobaltate(III)
7. Chloropentammincobalt(III) chloride
8. Bis(acetylacetonato)copper(II)
9. Hexaminenickel(II) chloride
10. Bis(thiocynato)pyridinemanganese (II)

d. Separation of a mixture of two metal ions by paper chromatography.

Separation of zinc and magnesium on a cation exchanger.

TEXTBOOKS:

1. A.L. Vogel, Text book of Inorganic quantitative analysis, ELBS, Third edition, 1976.
2. G.S.Vehla, Vogel's text book of Macro and Semimicro Qualitative Inorganic Analysis, fifth edition, Revised, 1979.
3. Douglas A.Skoog, F. James Holler. Stanley R Crouch, Principles of Instrumental Analysis, third edition 2007.

**COREPRACTICAL –III
PHYSICAL CHEMISTRY PRACTICAL-I**

SUBJECT CODE: 19PCHE307P	PRACTICAL	MARKS:100
SEMESTER:II	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To understand and verify the concepts and equations in physical chemistry by carrying out suitable experiments. Typical list of possible experiments are given. A minimum of 10– 12 experiments have to be performed.

EXPERIMENTS

1. Study of the adsorption of acetic acid or oxalic acid on charcoal,
verification of Freundlich isotherm and determination of concentration

- of given acetic acid or oxalic acid.
2. Construction of phase diagram for a simple binary system; naphthalene–biphenyl, naphthalene–p-dichloro benzene, naphthalene–diphenylamine.
 3. Construction of phase diagram for the three component system (partially miscible liquid system) acetone–chloroform–water; chloroform – acetic acid – water.
 4. Determination of the equilibrium constant of the reaction between iodine and potassium iodide by partition method.
 5. Determination of the concentration of given potassium iodide solutions by partition method.
 6. Determination of molecular weight of benzoic acid in benzene and the degree of association of benzoic acid in benzene using partition method.
 7. Kinetic study and comparison of rate constant for the inversion of cane sugar in presence of acid using polarimeter.
 8. Kinetic study of the reaction between acetone and iodine in acidic medium and determination of the order with respect to iodine and acetone.
 9. Kinetic study of saponification of ethyl acetate by sodium hydroxide conductometrically and determination of order of the reaction.
 10. Kinetic study and comparison of acid strength using acid catalysed hydrolysis of methyl acetate.
 11. Determination of temperature coefficient and energy of activation for the acid catalyzed hydrolysis of methyl acetate.
 12. Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide.
 13. Study of the primary salt effect on the kinetics of oxidation of iodide by persulphate
 14. Kinetic study of the decomposition of sodium thiosulphate by mineral acid.

REFERENCE

1. B.Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Published by viva books,2 012.
2. B.D.Khosla, V.C. Garg and A. Khosla, Senior Practical Physical

chemistry, R.Chand & Co New Delhi, 2011.

3. P.S. Sindu, Practical Physical chemistry-A modern Approach ,MacMillan India Ltd, first edition, 2006.
- 4.C.W.Garland, J.W. Nibler and D.P. Shoemaker Experiments in Physical Chemistry, Tata McGraw-Hill, New York, eighth edition, 2003.
5. A.M. Halpern, G.C. McBane, Experiments in Physical Chemistry, W.H. Freeman & Co, New York. Third edition, 2003.

**ELECTIVE-I
NATURAL PRODUCTS**

SUBJECTCODE:19PCHE311	THEORY	MARKS:100
SEMESTER:II	CREDITS:3	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To create awareness about the chemistry of biomolecules and their reactions.

UNIT-I: Nucleic acids (9 hrs)

Pyrimidine and purine bases- synthesis of Adenine, Cytosine, Thymine, Guanine and Uracil - structure and role of nucleic acid – nucleotide, nucleoside and poly nucleotides – DNA and RNA– structure, types – biological functions– genetic code.

UNIT-II: Proteins and Steroids (9hrs)

Proteins-classification-Merrifield synthesis- end group analysis -structure-biological function. Steroids -Diel's hydrocarbon, synthesis of bile acid. Structural elucidation of cholesterol-Conversion of cholesterol into estrone, testosterone and progesterone

UNIT-III: Terpenoids and Carotenoids (9hrs)

Classification, occurrence, general methods of determining structure-isoprene rule. Synthesis of the following molecules–camphor, terpineol, α and β -Carotene, lycopene.

UNIT-IV: Alkaloids and Anthocyanins (9hrs)

Total synthesis of cocaine, morphine and reserpine. Flavones, isoflavones, anthocyanins (Synthesis only)

UNIT- V: Bio synthesis (9 hrs)

General principles involved in the biosynthesis of amino acids, alkaloids, steroids and terpenoids. Bio synthesis of cholesterol, phenanthrene, alkaloids and bile acids.

TEXTBOOKS:

1. I.L. Finar, Organic chemistry, Vol- II, ELBS Publication, fifth edition, 1986.
2. O.P. Agarwal, Organic Chemistry of Natural Products, Krishna Prakashan Media Pvt. Ltd, forty second edition, 2011.
3. Gurdeep R. Chatwal, Organic chemistry of Natural products, Himalaya Publishing House, 2005.
4. L.A. Pacquette, Principles of Modern Heterocyclic Chemistry, Benjamin Cummings Publishing Co, London, 1978.

Question paper pattern:

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Section A	MCQ:1-10 , Fill up : 11-15 , T/F:16-20 Answer all questions	1 – 20	1	20
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Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTAL MARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit– 1	4	
	Unit– 2	4	
	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	2	
	Unit– 2	1	
	Unit– 3	2	
	Unit– 4	2	
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

SEMESTER - III

**CORE THEORY-8
SPECTROSCOPY-I**

SUBJECT CODE: 19PCHE312	THEORY	MARKS:100
SEMESTER:III	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To introduce the concept of interaction of matter with electromagnetic radiations leading to rotational, vibrational, electronic transitions.
- To learn the structural determination of both organic and inorganic compounds.

UNIT-I:Rotational, Vibrational and Raman Spectroscopy (15hrs)

Interaction of radiation with matter, Einstein coefficients, transition probability, Beer-Lambert law and absorbance .Rotational spectroscopy of rigid rotor, non-rigid rotor-diatomic and polyatomic molecules–Stark effect. Vibrational spectroscopy-harmonic oscillator-anharmonicity- vibrational spectra of polyatomic molecules- overtones, combination of bonds -vibrational coupling- Fermi resonance. IR spectra of poly atomic molecules-factors affecting the vibrational frequencies– Effect of hydrogen bonding and solvent effect - finger print region -identification of functional groups. FTIR, Raman spectra – rotational and vibrational Raman spectra– selection rules–Polarization of transitions – resonance Raman spectra.

UNIT-II: Applications of IR, Raman Spectroscopy (10 hrs)

Determination of bond length, force constant, vibrational frequency. Applications involving isotopic substitution. Determination of structure of organic compounds using IR absorptions. Applications of Infrared and Raman spectroscopy to inorganic systems-metal complexes, organometallic and simple inorganic compounds with special reference to coordination sites, isomerism etc., inorganic structure determination.

UNIT-III: Electronic spectroscopy (10hrs)

Electronic spectra of diatomic and polyatomic molecules -Frank-Condon principle – determination of dissociation energy – pre dissociation spectra-selection rules-types of electronic transitions – effect of conjugation and solvent - chromophores, auxochromers, Bathochromic and Hypsochromic shifts. Term symbols for electronic states of H₂ molecule. Applications in organic structure

determination—Woodward-Fieser rule for conjugate systems and unsaturated ketones – Scott rules for aromatic ketones. Optical rotatory dispersion and its application. Cotton effect, axial halo ketone rule and octant rule.

UNIT–IV:Applications of Electronic Spectra (15 hrs)

Term states of d^n ions - Term Symbols - Characteristics of d-d transitions - electronic spectra of coordination compounds - selection rules - band intensities and band widths - energy level diagrams of Orgel and Tanabe-Sugano-spectra of Ti^{3+} , V^{3+} , Ni^{2+} , Cr^{3+} , Co^{2+} , Cr^{2+} and Fe^{2+} calculation of $10Dq$ and B for $V^{3+}(\text{oct})$ and $Ni^{2+}(\text{oct})$ complexes. Charge transfer spectra -classification, mechanisms and interpretation with suitable examples. Applications of UV-Visible spectroscopy to inorganic and organometallic compounds with regard to structural elucidation.

UNIT V: Photo electron and NQR Spectra (10 hrs)

Photoelectron spectroscopy – basic principles UPS and XPS – photoelectron spectra-Koopmann's theorem- fine structure in PES, applications of UPS and ESCA- Introduction –Chemical shift and Correlation with electronic charges. ESCA - satellite peaks, spectral splitting, instrumentation, applications; Auger electron spectroscopy. Determination of dipole moment, NQR spectroscopy – theory of NQR – instrumentation – nuclear quadrupole coupling constants –applications.

REFERENCEBOOKS:

1. R.S.Drago, Physical Methods in Chemistry, Thomson learning, 1977.
2. Drago R.S, Physical Methods for Chemists, Saunders, (W.B), Co.Ltd, second edition, 1992.
3. Ebsworth E.A.V, DWA Rankin and C. Craddock, Structural methods in inorganic chemistry, Blackwell Science Inc. second edition, 1987.
4. Kemp.W, Organic Spectroscopy, Palgrave third edition, 2008.
5. Kalsi P.S., Spectroscopy of Organic compounds, New Age International Publication, fourth edition, 1999.
6. Pavia D.L. and Chapman G. M. Introduction to Spectroscopy, Books / Cole, fourth edition, 2008.
7. Christian G.D., Analytical Chemistry, Wiley, sixth edition, 2004.
8. Silverstein, Basseler and Morrill, Spectroscopic Identification of Organic Compounds, John Wiley & Sons, New York, fifth edition, 1991.
9. Sharma B.K., Instrumental methods of analysis, Goel Publication, twenty fourth edition, 2005.
10. Skoog D.A., Instrumental methods of analysis-Saunders College Publication, third edition, 2007.

11. R.M.Silverstein, Francis X- Webster, Spectroscopic Identification of Organic Compounds, Wiley student edition, New York. sixth edition, 2014.

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	Unit– 5	4	
Section B	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	1
	Unit– 4	1	1
	Unit– 5	1	1
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

CORETHEORY-9
SYNTHETIC METHODOLOGY

SUBJE CT CODE: 19PCHE313	THEORY	MARKS:100
SEMESTER:III	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To introduce the basic methodology for the synthesis of organic compounds.

UNIT-I: Modern Synthetic Methodology (15 hrs)

Retro synthetic analysis-disconnections- Synthons :Donors & acceptor and their synthetic equivalent- FGI-FGA-UMPOLUNG. Formation of C-C bond using alkylation and acylation of enamines, enolates, active methylene compounds and Organometallic compounds - RMgX , R_2LiCu , RLi with special reference to synthesis of 1,2 - 1,3 - 1,4 - 1,5- and 1,6 - dicarbonyl compounds. Synthesis of unsaturated carbonyl compounds using aldol condensation, Claisen reaction and Michael reaction - Cyclisation methods- Robinson annulations. Formation of C=C bond using Wittig and modified Wittig reactions. Role of sulphur ylides and rearrangements (Pinacol-Pinacolone and Favorski rearrangement) inorganic synthesis. Protection and deprotection of functional groups (-OH, - NH_2 , C=O, -COOH).

UNIT-II: Synthetic Reagents (15 hrs)

Reagents used for oxidation- TPAP, Dess-martin, silver carbonate / molecular sieves and CAN. Reagents used for Reductions- $(\text{PPh}_3)_3\text{RhCl}$, Lindlar catalyst, 9-BBN, chiral boranes, NaBH_3CN , DIBAL and selectrides - Birch reduction (Hetero cyclic compound). Role of Bu_3SnH , trimethyl silyl chloride, LDA and dithiane in organic synthesis.

UNIT-III: Synthetic Applications of Name Reactions (10 hrs)

Sandmeyer reaction, Ullmann reaction, Gomberg reaction, Pschorr reaction, Hunsdicker reaction. Heck reaction, Suzuki coupling, McMurry

olefination, Prins reaction, Ritter reaction, Mitsunobu reaction, Sharpless asymmetric epoxidation, Kumada coupling, Negishi coupling, Stille coupling and Sonogashira coupling.

UNIT-IV: Synthesis of Target Molecules (10 hrs)

Retrosynthetic analysis, donor and acceptor synthons- examples and synthesis of target molecules - 5-hexenoic acid, bicyclo (4, 1, 0) heptane-2-one, trans-9-methyl-1-decalone, Cubane, longifolene, cis -jasmone and onocerin.

UNIT-V: Green Chemistry (10 hrs)

Green chemistry and atom economy principle- Use of ionic liquids and molten salts inorganic synthesis – role of Microwave irradiation and ultrasound waves in organic synthesis (microwave assisted reactions–Hofmann elimination, Hydrolysis reactions, Fries rearrangement, Diels-alder reaction, Oxidation reactions, Decarboxylation, Reactions without using solvents)–zeolites in synthesis.

REFERENCE BOOKS:

1. William Caruthers and Coldham, Modern methods of organic synthesis, Cambridge Univ, Press, fourth Edition, 2010.
2. Ratan Kumar Kar, Frontier Orbital and Symmetry Controlled Pericyclic reaction, Books & allied Pvt.Ltd, first Edition, 2010.
3. I.L. Finar, Organic chemistry Vol-II, Pearson Education Pvt. Ltd, fifth edition, 2005.
4. Stuart Warren, Organic synthesis - The Dis connection approach, John Wiley (P) Ltd, Reprint 2011.
5. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part-A and Part-B, Plenum Press, New York, fifth edition, 2015.
6. J. March, Advanced Organic Chemistry, John Wiley & sons, Singapore, fourth edition, 1992.
7. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press, second edition, 2014.
8. Rashmi Sanghi and M.M. Srivastava, Green Chemistry, Narosa Publishing House Pvt. Ltd, fifth edition, 2012.
9. V.K. Ahluwalia, Green Chemistry-Greener alternative to synthetic

- organic transformation, Narosa publishing house Pvt. Ltd, first edition, 2011.
10. J.P. Tierney and P. Lidstrom, Microwave Assisted Organic Synthesis, Wiley India Pvt. Ltd, first edition, reprint, 2009.
 11. R.O.C Norman and J.M. Coxon, Principles of organic synthesis, CRC press, third edition, 2012.
 12. Ratan Kumar Kar, Fundamentals of organic synthesis—the retrosynthetic analysis vol-2, New central book agencies first reprint, 2008.
 13. Michael B. Smith, Organic synthesis, McGraw Hill, (Singapore) second edition, 2002.

Question paper pattern:

Section	Question Component	Numbers	Marks	Total
Section A	MCQ:1-10 , Fill up : 11-15 , T/F:16-20 Answer all questions	1 – 20	1	20
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Section C	Essay Answer any 3 out of 5 questions	29– 33	15	45
TOTAL MARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
		Theory	Problems
Section A	Unit– 1	4	
	Unit– 2	4	
	Unit– 3	4	
	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	1	1
	Unit– 2	1	
	Unit– 3	1	1
	Unit– 4	1	1
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

CORE THEORY-10
THERMODYNAMICS AND ELECTRO CHEMISTRY

SUBJECT CODE: 19PCHE314	THEORY	MARKS:100
SEMESTER:III	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To understand and appreciate the significance and applications of classical, statistical thermodynamics and solution electro chemistry.

UNIT-I: Thermodynamics – I (10 hrs)

Partial molar properties – Partial molar free energy (chemical potential)- Partial molar volume- partial molar heat content- their significance and determination of these quantities-variation of chemical potential with temperature and pressure.

Thermodynamics of real gases - gas mixture-fugacity definition- determination of fugacity – variation of fugacity with temperature and pressure- thermodynamics of ideal and non ideal binary solutions - dilute solutions-excess functions for non ideal solutions and their determination-the concepts of activity and activity co-efficient- determination of standard free energies- choice of standard states- determination of activity and activity coefficient for non electrolytes.

UNIT-II: Thermodynamics-II (10 hrs)

Concept of thermodynamic probability-distribution of distinguishable and non distinguishable particles. Maxwell-Boltzmann, Fermi-Dirac and Bose - Einstein statistics- Modes of contribution to energy. Partition function – Translational, vibrational and rotational partition functions for mono, diatomic and poly atomic ideal gases.

UNIT-III: Thermodynamics – III (10 hrs)

Thermodynamic functions in terms of partition functions-equilibrium constant for isotope exchange and dissociation of diatomic molecules- heat capacity of solids (Einstein and Debye models) - ortho and para hydrogen-Planck's radiation law – electron in metals.

UNIT-IV: Electro chemistry of Solutions (15 hrs)

Ion-solvent interaction-Born's treatment (structureless continuum model

only, no derivation); ion- ion interaction-Mean ionic activity and activity coefficient-concept of ionic strength -Debye- Huckel theory of strong Electrolytes-Derivation of Debye-Huckel limiting law validity of the equation -Debye-Huckel limiting law at low and appreciable concentration of the electrolytes-qualitative and quantitative verification-Deby-Huckel- Bronsted equation.

Ion transport- theory of strong electrolytes for electrolytic conductance-derivation of Onsager equation-validity of the equation-modification of Onsager equation. Ion association -Bjerrum treatment of association-Bjerrum ion association constant-factors influencing ion association-effect of ion association on conductivity and activity coefficient of electrolytes in solution.

UNIT–V: Dynamic Electro chemistry(15 hrs)

The electrode-electrolyte interface-electrical double layer-IHP-OHP-contact adsorption-surface excess and its importance-Thermodynamics of electrified interface-electro capillary phenomenon-Lippmann equation, Lippmann potential-polarizable and non-polarizable interface. Structure of double layer- Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer. Electro kinetic phenomena (Electrophoresis, electroosmosis, sedimentation potential and streaming potential – concepts only) derivation of Butler-Volmer equation for one step electron transfer reactions, Tafel equation-significance of exchange current density and symmetry factor. Polarization and over potential-Abriefac count of Hydrogen over potential-factors affecting Hydrogen over potential-mechanism of hydrogen evolution and oxygen evolution-concentration polarization.

Corrosion: Theories, types, prevention and applications of corrosions. Fuel Cells - hydrogen - oxygen fuel cell, construction and applications.

TEXTBOOKS:

1. J.O.M. Bokris and A.K.N. Reddy, Electro chemistry, Vol 1&2, Kluwer academic/Plenum publishers, New York, Second edition. 2002.
2. S. Glasstone, Introduction to Electro chemistry, Liton educational Publishing INC, reprint 2010.
3. D.R. Crow, Principles and Applications of Electrochemistry, Chapman and Hall, fourth edition, 1994.
4. M.C. Gupta, Statistical thermodynamics, Wiley, Eastern, New Delhi, reprint, 2009.
5. B.C Mc Clellan and Statistical thermodynamics, Chapman and Hall, London.1973.
6. Nester Perez, Electrochemistry and corrosion science, Springer London, reprint, 2010.
7. K.L. Kapoor, Physical chemistry, MacMillan India Ltd, third edition, 2009

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	Unit– 4	4	
	Unit– 5	4	
Section B	Unit– 1	1	1
	Unit– 2	1	
	Unit– 3	1	1
	Unit– 4	1	
	Unit– 5	1	1
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

ELECTIVE-II
SOLIDSTATEANDNANOCHEMISTRY

SUBJECT CODE: 19PCHE317	THEORY	MARKS:100
SEMESTER:III	CREDITS:3	TOTAL HOURS: 60

COURSE OBJECTIVES:

- Intended to reveal the thorough learning of solid state chemistry and Nano materials and their applications.

UNIT-I: Solid State Chemistry (15hrs)

Classification of crystals and elements of symmetry (including glide planes and screw axis) Bravais lattices; planes and indices, packing of crystals – bcc, fcc and hcp -volume occupied in bcc, fcc and hcp. X-ray diffraction and Bragg's law, powder diffraction -Debye Scherrer method, refinement and structure solution of some compounds, Indexing with JCPDS, FWHM and its application. Miller Indices, Point groups, stereographic projection of 32 point groups and space groups, isogonal symmetry groups and reciprocal lattice. Single Crystal Analysis and its Applications. - Structural aspects of rock salt, rutile, fluorite, antiferite, zinc blende, wurtzite, cristobalite, spinels, inverse spinels and silicates.

Electronic structure of solids - band theory, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, synthesis and purification of semiconducting materials. Inorganic phosphors-synthesis and applications. LED, FED – an introduction, Photoconductors, photovoltaic cells, solar batteries. Lasers-introduction and types, Inorganic laser - Ruby, Nd: YAG laser -instrument and principle.

UNIT-II: Imperfection in Crystals (10 hrs)

Perfect and imperfect crystals, lattice defects-types of defects. Order and disorder phenomena, thermodynamics of Schottky and Frenkel defect formation, Determination of defects. Non-stoichiometric defect and incorporation of stoichiometric excess defects (structural and thermodynamic aspects).Phase transitions, diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion.

UNIT-III: Magnetic Properties of Solids (15 hrs)

Introduction, magnetization, electron spin and magnetic moment, types of magnetism and materials – examples and applications. Theory of diamagnetism and paramagnetism. Langevin's theory (Derivation not required) - paramagnetic susceptibility of solids. Temperature independent paramagnetism - spin cross over phenomena. determination of magnetic susceptibility by Gouy and Faraday method.

Domain theory – Hysteresis Loop – applications. Properties of perovskite and magneto-plumbites- Hard and Soft magnetic materials- Super conductors – superconductivity in metals, alloys and ceramics materials (mixed oxides)- BCS theory, Meissner effect, type I and II superconductors, application-Fullerenes as super conductors.

UNIT-IV: Nanomaterials - Synthesis, Characterization and Properties (10 hrs)

Introduction to Carbon based nanomaterials, Metal based materials, dendrimer sand composites. Classification of nano materials based on dimensions. Properties of nano materials-size dependent properties-mechanical, physical and chemical properties. Quantum effects. Synthesis of nanomaterials : bottom up and top down method. Introduction on synthesis of nanomaterials via thermal, ball milling, Laser ablation, colloidal, sol-gel, chemical vapour deposition and electrochemical method. Characterization methods of nanomaterials: scanning electron microscopy (SEM) for morphology, Atomic Force microscopy (AFM), Transition Electron Microscopy (TEM) -Crystallite size and SAED pattern.

UNIT-V: Application of Nanomaterials – basic introduction (10 hrs)

Energy-fuel cells, Microbial fuel cell, hydrogen storage, nano phosphors for High - Definition TV, Next-Generation Computer Chips, Quantum electronic devices- CNT based applications and Field Emission Display - Biochemical sensor. Environmental - Membrane based water purification. Catalysis-organic transformation and photo catalysis. Biological applications –diagnostic and imaging, targeted drug delivery, theranostic reagents, Nano coatings and paintings. Cosmetic applications. Disadvantages of Nano materials–Nano toxicity.Green Nano chemistry.

REFERENCEBOOKS:

1. A.R. West, Basic Solid State Chemistry, John Wiley, second edition,1999
2. W. E. Addison, Structural Principles in Inorganic Chemistry, Longman,1961,
3. M. Adams, Inorganic Solids, John Wiley Sons,1974
4. M. Wilson, K. Kannangara, G Smith, M. Simmons, B. Raguse,
Nanotechnology: Basic science and Emerging technologies, Overseas Press
India Pvt. Ltd, New Delhi, First Edition, 2005.
5. C.N.R. Rao, A. Muller, A.K. Cheetham(Eds), The chemistry of
nanomaterials : Synthesis, properties and applications, Wiley VCH,
Wein heim, 2004.
6. Kenneth J. Klabunde (Eds), Nanoscale Materials Science, John
Wiley&Sons,Inc.,2001.
7. C.S.S.R. Kumar, J. Hormes, C.Leuschner, Nano fabrication
towards biomedical applications,Wiley–VCH Verlag GmbH
&Co, Weinheim, 2004.
8. W.Rainer, Nano Electronics and informationTechnology,Wiley,2003.
9. K.E. Drexler, Nanosystems,Wiley,1992.
10. G.Cao, Naostructures and Nanomaterials: Synthesis, properties and
applications, Imperical College Press, 2004.

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	Unit- 3	2	
	Unit- 4	2	
	Unit- 5	1	
Section C	Unit- 1	1	
	Unit- 2	1	
	Unit- 3	1	
	Unit- 4	1	
	Unit-5	1	

SEMESTER - IV

**CORE THEORY-11
PHOTOCHEMISTRY**

SUBJECT CODE: 19PCHE318	THEORY	MARKS:100
SEMESTER:IV	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To deal with the theory and the applications of photochemistry in explaining various organic and inorganic reactions.

UNIT-I: Fundamentals (15 hrs)

Absorption and emission of radiation-Frank-Condon principle- Physical properties of electronic excited molecules - Spin multiplicity - Singlet and triplet excited states - decay of electronically excited states - radiative and non- radiative processes-fluorescence and phosphorescence- Spin forbidden non-radiative transitions-internal conversion and inter system crossing - energy transfer process - excimers and exciplexes-delayed fluorescence and phosphorescence - Triplet-Triplet annihilation - static and dynamic quenching-Stern - Volmer analysis. Quantum efficiency-quantum yield - sensitization and sensitizer - allowed- forbidden process-Molecular structure and photo physical and photo chemical reactivity

UNIT-II: Techniques and Photochemical Reactions (10 hrs)

Quantum yield measurements - Flash photolysis techniques - Actinometry-quantum yield of photo physical process and photochemical reactions. Life time measurements – steady state and non-steady state methods. Fluorescence spectroscopy–principle-instrumentation and applications. –fluorescence based sensors.

UNIT-III: OrganicPhoto chemistry (10 hrs)

Photo chemistry of ketones – Norrish Type-I, Norrish type –II - Photo reduction, - photochemistry of olefins - cis –trans isomerisation - Photocyclo addition, - Paterno – Buchi reaction –photo chemistry of aromatic compounds – photo rearrangements - Di- π methane rearrangement, Barton reaction and Photo Fries reaction– Photochemistry of cyclo hexadienones–photochemistryof santonin-synthesis of Vitamin D.

UNIT-IV: Photochemistry of Co-ordination Compounds (10 hrs)

Types of Photo chemical reaction–photo isomerisation, photo substitution and photo redox reactions of Cobalt, Chromium, Platinum and Ruthenium

complexes. - photo voltaic cells and photo galvanic cells- solar energy conversion- photo electrochemistry- Role of Ruthenium bipyridine [Ru(bpy)₃] complexes in solar energy conversion- photosynthesis.

UNIT–V:Applied Photo chemistry (15 hrs)

The solar spectrum, antennae, reaction centers, photo processes in organic, inorganic, and sensitized solar cells- Excitons, polarons, solitons, semiconductor junctions, photocurrent and photovoltage, photo catalysis, photodamage and repair, DNA photo dynamic therapy, photochemical process in the environment, photochemical process in medicine and in the pyrotechnics-photo degradation of polymers- photochemistry of vision.

TEXT BOOKS:

1. N.J. Turro, Modern Molecular Photochemistry (MMP), University Press, Menlo Park, CA, 1978.
2. A.Gilbert and J. Baggott, Essentials of Molecular Photochemistry, CRC Press, London, UK, 1991.
3. J. Mattay and A.Griesbeck, eds., Photochemical Key Steps in Organic Synthesis, VCH, New York, 1994.
4. J.D. Coyle, ed., Photochemistry in Organic Synthesis, Royal society of Chemistry, London, 1986.
5. K.K. Rohatgi Mukherjee, Fundamentals of photochemistry, New Age International Pvt. Ltd, reprint 2008.

REFERENCE BOOKS:

1. W.H. Horspool, ed., Synthetic Organic Photochemistry, Plenum, New York, 1984.
2. I. Ninomiya and T.Naito, eds., Photochemical Synthesis, Academic Press, London, 1989.
3. J.C. Scaiano, ed., CRC Handbook of Organic Photo chemistry, vol.1 and 2, CRC Press, Boca Raton, Florida, 1989.

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Section B	Unit– 1	2	
	Unit– 2	1	
	Unit– 3	1	1
	Unit– 4	2	
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

**CORE THEORY-12
SPECTROSCOPY-II**

SUBJECT CODE: 19PCHE319	THEORY	MARKS:100
SEMESTER:IV	CREDITS:4	TOTALHOURS: 60

COURSE OBJECTIVES:

- To learn the principles of NMR, ESR & mass spectrometry and its applications to organic and inorganic compounds.

UNIT-I: Magnetic Resonance Spectroscopy (10 hrs)

Nuclear magnetic resonance spectra: Theory- the nuclear spin, Larmor frequency, NMR isotopes, population of nuclear spin levels- relaxation processes. Chemical shift- shielding constant, diamagnetic anisotropic influence - ring currents – diatropy and paratropy. Spin-spin interaction - low and high resolution spectra. Nuclear magnetic double resonance- nuclear Overhauser effect-Fourier transform technique-¹³C-NMR (elementary treatment).

UNIT-II: Applications of NMR Spectroscopy to Organic Compounds (10 hrs)

Proton NMR applications to structure elucidation of simple organic molecules - chemical shift values of various chemically non-equivalent protons and correlation to protons bonded to carbon and protons bonded to other nuclei - chemical exchange, effect of deuteration. First order PMR spectra - complex spin-spin interaction between two, three, four and interacting nuclei, virtual coupling, simplification of complex spectra using shift reagents - coupling constant -variation of coupling constant with dihedral angle, Karplus curve. ¹³C-NMR applications to structure elucidation of simple organic molecules – complete decoupled CMR – off resonance spectra- chemical shift values. Elementary treatment of two-dimensional NMR spectroscopy, NOESY, COSY, and DEPT.-Conjunct problems based on IR, Mass and NMR data.

UNIT-III: Applications of NMR Spectroscopy in Inorganic Chemistry (10 hrs)

Applications of ³¹P, ¹⁹F, ¹¹⁹Sn and ¹⁹⁵Pt NMR spectroscopy in the structural assessment of simple inorganic compounds. Inter and intra molecular exchange studies using NMR. Applications of NMR in the study of coordination complexes and organo metallic derivatives. Applications of NMR in the study of trans effect and fluxional behavior of inorganic molecules and complexes.

UNIT-IV: Applications of ESR Spectra and Mossbauer Spectra (15 hrs)

ESR spectra of transition metal complex -copper, manganese and vanadyl complexes. Applications of ESR spectroscopy based on number of ESR signals, multiplicity, anisotropy, magnitude of g values and A values – Covalency of complexes. Applications of ESR in the study of bio-inorganic molecules. Mossbauer spectroscopy – principle – instrumentation – recoil energy – Doppler effect – number of MB signals – isomer shift – quadrupole splitting – magnetic splitting. Applications of ^{57}Fe , Sn^{119} and I^{129} Mossbauer spectra.

UNIT-V: Mass Spectrometry (15 hrs)

Principle – instrumentation – isolation techniques - EI, CI, FD, FAB, SIMS - presentation of spectral data – molecular ions – determination of molecular mass – Isotopic peaks - determination of molecular formula – Meta stable peaks. Fragmentation – nitrogen rule, Mc Lafferty rearrangement – Retro Diels–Alder fragmentation – interpretation of mass spectra of hydrocarbons, alcohols, phenols, aldehydes, ketones, carboxylic acids, amines and their derivatives. Identification of organic compounds using mass spectrometry – problems.

REFERENCE BOOKS:

1. C.N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy, Tata Mc Graw-Hill, New Delhi, fourth edition, 2010.
2. D.A. McQuarrie and J.D. Simon, Physical Chemistry-Molecular approach, Viva students Ed, reprint, 2010.
3. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, John Wiley, fifth edition, 1997.
4. R.S. Drago, Physical Methods in Chemistry, Saunders College Publishers, 1977.
5. R.V. Parish, NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Horwood, New York, 1990.
6. E.A.V. Ebsworth and D.W.H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry Blackwell scientific, Oxford, 1987.
7. D.L. Pavia, G.M. Lampman, G.S. Kriz and J.R. Vyan, Introduction Spectroscopy, Cengage Learning, Indian edition, 2008.
8. R. M. Silverstein, F. X. Webster, Spectrometric Identification of Organic Compounds Wiley India, sixth edition, reprint, 2011.
9. G.C. Levy, R.L. Lichter, G.L. Nelson, ^{13}C NMR Spectroscopy, Wiley, 1992.
10. D.H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw Hill, 2008.
11. Anees A. Siddiqui, Mass Spectrometry, CBS Publishers, first edition, 2011.
12. R.J. Abraham, J. Fisher and P. Loftus, Introduction to NMR spectroscopy - Wiley, 2005.
13. John.R. Dyer, Application of absorption spectroscopy of organic compounds, Prentice–Hall of India Pvt. Ltd, fifth edition, 1984.

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TOTAL MARKS				100

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	Unit– 4	1	1
	Unit– 5	1	
Section C	Unit– 1	1	
	Unit– 2	1	
	Unit– 3	1	
	Unit– 4	1	
	Unit-5	1	

CORE PRACTICAL –4
ELECTRO ANALYTICAL PRACTICAL

SUBJECTCODE: 19PCHE315P	PRACTICAL	MARKS:100
SEMESTER:IV	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To help the students to understand and apply the concepts of electro analytical chemistry.

UNIT–I: Conductometric Experiments

1. Determination of equivalent conductance of strong electrolytes and verification of Debye-Huckel-Onsager equation.
2. Determination of dissociation constant of weak electrolyte using Ostwald's dilution law.
3. Conductometric Titration between simple and mixture of strong and weak acids and base and precipitation titration involving a single halide.

UNIT–II: Potentiometric Experiments

1. Determination of pH and calculation of pKa.
3. Determination of solubility product of sparingly soluble salt.
4. Potentiometric titrations between simple and mixture of strong and weak acids and Base.
5. Redox Titrations by EMF measurements
6. Precipitation titration of mixture of halides by EMF measurements.

UNIT–III: Colorimetric Experiments

1. Photoelectric method: Estimation of Iron, Nickel, Manganese and Copper.
2. Determination of Cr^{2+} and Mn^{2+} ions present in water sample by Colorimetry.

REFERENCE

1. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva books, 2012.
2. B.D. Khosla, V.C. Garg and A. Khosla, Senior Practical Physical chemistry, S.Chand and Co., New Delhi, 2011.
3. P.S. Sindu, Practical Physical Chemistry-A modern Approach,

MacMillan India Ltd, first edition, 2006.

4. C.W. Garland, J.W. Nibler and D.P. Shoemaker, Experiments in Physical Chemistry, Tata McGraw-Hill, New York, eighth edition, 2003.
5. A.M. Halpern, G.C. Mc Bane, Experiments in Physical Chemistry, W.H. Freeman & Co, New York. Third edition, 2003.

ELECTIVE PRACTICAL-I
ANALYTICAL CHEMISTRY PRACTICAL

SUBJECT CODE: 19PCHE316P	PRACTICAL	MARKS:100
SEMESTER:IV	CREDITS:4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To impart the techniques of analysis of ores and alloys; quantitative estimation of organic compounds and inorganic metal ions and spectral interpretations.

A. ESTIMATIONS (ANYFOUR):

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of glucose (Bertrand's Method)
4. Saponification of fat or oil.
5. Iodine value of an oil.

**B. SPECTRAL INTERPRETATION OF ORGANIC COMPOUNDS-
UV,IR,PMR AND MASS SPECTRA**

1. 1,3,5-Trimethyl benzene
2. Pinacolone
3. Benzyl bromide
4. Phenyl acetone
5. Isopropyl alcohol
6. 2-N,N-Dimethyl amino ethanol
7. 4-Picoline
8. Cinnamaldehyde

C. SPECTRAL INTERPRETATION OF INORGANIC COMPOUNDS

1. ^{31}P NMR Spectra of methyl phosphate
2. ^{31}P NMR Spectra of HPF_2

3. ^{19}F NMR Spectra of ClF_3
4. ^1H NMR Spectra of Tris (ethylthioacetoacetato)cobalt(III)
5. Expanded high resolution NMR spectra of
(N- propyl isonitroso acetylacetonato iminato)
(acetylacetonato)Nickel(II)
6. ESR Spectra of the aqueous $\text{ON}(\text{SO}_3)_2^{2-}$ ion.
7. ESR Spectra of the H atoms in CaF_2
8. ESR Spectra of the $[\text{Mn}(\text{H}_2\text{O})_6]^{2+}$ ion
9. ESR Spectra of the bis(salicyladiminato)copper (II)
10. IR Spectra of the sulphato ligand
11. IR Spectra of the nitro and nitropentaminecobalt(III) chloride
12. IR Spectra of the dimethylglyoxime ligand and its Nickel(II) complex.
13. IR Spectra of carbonyls
14. Mossbauer spectra of $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$
15. Mossbauer spectra of FeCl_3
16. Mossbauer spectra of $[\text{Fe}(\text{CN})_6]^{3-}$
17. Mossbauer spectra of $[\text{Fe}(\text{CN})_6]^{4-}$

D. QUANTITATIVE ANALYSIS OF COMPLEX MATERIALS

To impart the techniques of analysis of alloys; preparation and analysis of inorganic complexes.

a) Analysis of Alloys:

1. Analysis of copper and nickel from cupro-nickel alloy.
2. Estimation of copper and zinc in brass.
3. Estimation of iron and nickel in stainless steel.
4. Estimation of iron and magnesium from the mixture.

b) Analysis of Inorganic Complex Compounds :(for internal assessment only)

1. Preparation of cis and trans potassium bis(oxalato)diaquochromate and analysis of each of these for chromium.
2. Preparation of potassium tris(oxalato)aluminate(III) and analysis for iron and oxalate.

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