

GURU NANAK COLLEGE (AUTONOMOUS)

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

Velachery Main Road, Velachery, Chennai – 600042.



M.Sc. Chemistry

(SEMESTER PATTERN WITH CHOICE BASED CREDIT SYSTEM)

Syllabus

(For the candidates admitted in the Academic year 2017-18 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 modernise 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 (2017-19) Batch

Semester	Course Component	Subject Code	Subject Name	Credits	Hours	CIA	ESE	Total
Semester – I	Core-1	16PCHEC01	Stereochemistry and Reaction Mechanism	4	5	50	50	100
	Core-2	16PCHEC02	Chemical Kinetics	4	4	50	50	100
	Core-3	16PCHEC03	Coordination Chemistry	4	4	50	50	100
	Core-4	16PCHEC04	Analytical Chemistry	4	4	50	50	100
	Core Practical-1	16PCHEC05P	Organic Chemistry Practical-1	*	5	*	*	*
	Core Practical-2	16PCHEC06P	Inorganic Chemistry Practical-1	*	4	*	*	*
	Core Practical-3	16PCHEC07P	Physical Chemistry Practical-1	*	4	*	*	*
	Soft Skill - 1	16PGSLS01	Essentials of Language and Communication	2		50	50	100
Total Credits: 18 / Total Hours per week: 30								
Semester – II	Core-5	16PCHEC08	Quantum chemistry and Group theory	4	5	50	50	100
	Core-6	16PCHEC09	Organometallics and Bioinorganic chemistry	4	4	50	50	100
	Core-7	16PCHEC10	Chemistry of Aromatic compounds and Concerted reactions	4	4	50	50	100
	Core Practical-1	16PCHEC05P	Organic Chemistry Practical-1	4	5	50	50	100
	Core Practical -2	16PCHEC06P	Inorganic Chemistry Practical-1	4	4	50	50	100
	Core Practical-3	16PCHEC07P	Physical Chemistry Practical -1	4	4	50	50	100
	Elective-1	16PCHEE01	Chemistry of Natural Products	3	4	50	50	100
	Soft Skill - 2	16PGSLS02	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	16PCHEC11	Spectroscopy-1	4	5	50	50	100
	Core-9	16PCHEC12	Synthetic Methodology	4	5	50	50	100
	Core-10	16PCHEC13	Thermodynamics and Electrochemistry	4	5	50	50	100
	Core Practical-4	16PCHEC14P	Electroanalytical Practical	*	5	*	*	*
	Elective Practical-1	16PCHEE02P	Analytical Chemistry Practical	*	5	*	*	*
	Elective-II	16PCHEE03	Solid State and Nano Chemistry	3	5	50	50	100
	Soft Skill-3	16PGSLS03	Managerial Skills	2	-	50	50	100
		16PINT401	Summer Internship **	2	-	50	50	100
Total Credits: 19 / Total Hours per week: 30								
Semester – IV	Core-11	16PCHEC15	Photochemistry	4	5	50	50	100
	Core-12	16PCHEC16	Spectroscopy-II	4	5	50	50	100
	Core Practical-4	16PCHEC14P	Electroanalytical Practical	4	5	50	50	100
	Elective Practical-1	16PCHEE02P	Analytical Chemistry Practical	4	5	50	50	100
	Soft skill-4	16PGSLS04	Spoken and Presentation Skills	2	-	50	50	100
		16PCHEC17	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 a 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 – 600 042

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

CORE – I
STEREOCHEMISTRY AND REACTION MECHANISM

SUBJECT CODE: 16PCHC01	THEORY	MARKS 100
SEMESTER: I	CREDITS: 4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- This course aims to explain basic concepts in stereochemistry 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-Newman and Sawhorse projection- interconversion of projection formulae- prochiral center- asymmetric synthesis-Cram's rule and Prelog's rule-optical purity – enantiomeric excess – stereospecific and stereoselective reactions.

Geometrical isomerism: E-Z nomenclature of olefins and oximes-Geometrical and optical isomerism of mono and disubstituted cyclopropane, cyclobutane, cyclopentane and cyclohexane derivatives- homotopic, enantiotopic and diastereotopic hydrogen - prochiral carbon (upto 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 disubstituted ethane derivatives- cyclopropane, cyclobutane, cyclopentane and cyclohexane derivatives- conformational free energy – conformational analysis of mono and disubstituted cyclohexanes and their stereochemical feature (geometrical and optical isomerism)-conformation and stereochemistry of decalin and 9 methyl decalin- conformation of glucose.

Conformation and reactivity: steric and product development control – reduction of tertiary butyl cyclohexanone by hydride – stereo chemistry of oxidation of cis & trans tertiary butyl

cyclohexanols by Cr (VI) – stereochemistry of the reaction between nitrous acid and α -amino cyclohexanols.

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

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 – neighboring 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 compounds, hydrolysis of esters, Claisen and Dieckmann condensations.

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

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- Simmons Smith reaction. Mannich, Stobbe, Darzen, Wittig, Wittig-Horner and Benzoin reactions. Nitrene: Methods for generating nitrenes and their reactions. (Stereochemical 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.

TEXT BOOKS:

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 interscience, sixth edition, 2007.
6. R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Organic chemistry, Pearson Prenticehall, seventh edition, 2012.
7. P.S. Kalsi, Organic reactions and their Mechanism, New Age International Ltd, third edition, 2012.

REFERENCE BOOKS:

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

CORE - 2
CHEMICAL KINETICS

SUBJECT CODE: 16PCHEC02	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: Chemical Kinetics-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: Chemical Kinetics-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: Chemical Kinetics-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: Chemical kinetics –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: Chemical kinetics –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 text book 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. Harnum, Chemical Kinetics, D.C. Health and Co. 1966.

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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	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	1a	
	Unit – 4	1b	
	Unit – 5	1	

CORE THEORY – 3
COORDINATION CHEMISTRY

SUBJECT CODE: 16PCHEC03	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, spectrochemical 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, TASSO, 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 distortions.

Unit II: Stability and stereo isomerism 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). Stereo chemical 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; atom 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, 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 - ligandfield 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, metalloboranes, and metallocarboranes- 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: polyphosphazene and cyclic aminophosphanes, 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. Day and 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, Transition metal Chemistry, Vol. 1 to 5, Academic Press, London, 1968.
2. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, Oxford Univ. press, New York, second edition.1994.

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

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	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	1a	
	Unit – 5	1b	

CORE THEORY – 4
ANALYTICAL CHEMISTRY

SUBJECT CODE: 16PCHEC04	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

(10 hrs)

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 and T tests. Calibrations – General idea of calibration, calibration of glasswares, balance, instruments and other equipments. Uncertainty in chemical analysis: theory, significance, sources of uncertainty and model calculations 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 (15 hrs)

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

Sampling of solid, liquid and gases – handling, collection, transport, storage - primary sample, laboratory sample, analytical sample.

Physico- chemical analysis of medicines (formulated), petrochemicals (fuels), ores, cement, fertilizers, alloys, organic compounds, packed foods, water and air. [Note: Any one representative example in each category and testing of important parameters only]

UNIT - III: Separation Techniques (10 hrs)

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

UNIT - IV: Electroanalytical Methods (15 hrs)

Polarography – Theory, Instrumentation, type of currents (includes kinetic & catalytic currents), advantageous of DME, half wave potential. Qualitative and quantitative applications to analysis of inorganic, organic compounds and determination of dissolved oxygen. Derivative Polarography – Amperometry and biamperometry (theory, equipment and applications).

Cyclic voltammetry – theory, instrumentation and applications to inorganic and organic systems. Application of CV in applied research viz., prediction of reaction mechanism, redox behavior of chemical compounds and identification of number of electrons in the electrochemical processes. Ion selective electrodes - theory and applications of potentiometry, conductometry and coulometric titrations.

UNIT - V: Thermal, Radio-analytical Methods and Computers in Chemistry (10 hrs)

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

Applications of computers in chemistry: Applications of software - Chemdraw, computational chemistry and molecular simulations.

TEXT BOOKS:

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 Text book of quantitative Chemical Analysis; Pearson Education Pvt.Ltd. sixth edition, 2004.

REFERENCE BOOKS:

1. E Prichard, Quality in the analytical chemistry laboratory, John Wiley and sons, 1997.
2. W Funk, V Dammann, G. Donnevert, 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 Asia Pvt., 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, Lynne L., 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, John Wiley, 1980.
8. S. M. khopkar, Environmental Pollution Analysis, New Age International publication, 2011.
9. Seonard' lCiacere, Water and water pollution (hand book), 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. Melon, 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; Inter science, 1966.
18. K.V. Raman, Computers in Chemistry, Tata McGraw-Hill Education Pvt. Ltd, tenth reprint 2008.

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TOTAL MARKS				100

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		Theory	Problems
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	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	1a	
	Unit – 4	1	
	Unit - 5	1b	

SEMESTER - II

CORE THEORY – 5
QUANTUM CHEMISTRY AND GROUP THEORY

SUBJECT CODE: 16PCHEC08	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 atoms in groundstate- Slater rules, Slater orbital and HFSCF methods- Born-Oppenheimer approximation-Valence Bond theory for hydrogen molecule – LCAO – MO theory for di and poly atomic 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: Group theory –II

(15 hrs)

Hybrid orbitals in non-linear molecules- (CH_4 , XeF_4 , BF_3 , SF_6 and NH_3). Symmetry based selection rules for infrared, Raman and electronic spectra of ethylene and formaldehyde-application of group theory.

TEXT BOOKS:

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.1988.
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.

REFERENCE BOOKS:

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., New York, 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:

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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
TOTAL MARKS				100

Distribution of Questions:

Sections	Units	No. of Questions	
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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	1a	
	Unit – 2	1b	
	Unit – 3	1	
	Unit – 4	1	
	Unit - 5	1	

CORE THEORY – 6
ORGANOMETALLICS AND BIOINORGANIC CHEMISTRY

SUBJECT CODE: 16PCHC09	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 and Study of Carbonyl compounds (10 hrs)

Valence electron count (16/18 electron rules); structure and bonding in mono and polynuclear metal carbonyls; substituted metal carbonyls and related compounds; synthesis and reactivity of metal carbonyls; Back bonding and synergic effect - π acids, vibrational spectra of metal carbonyls; dinitrogen and dioxygen as ligands in organometallic compounds.

UNIT – II: Reactions of organometallic complexes (15 hrs)

Types of M-C bonds; synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes; synthesis, structure and bonding of metallocenes and bent metallocenes; isolobal analogy. Association, Substitution, Addition, oxidative addition, reductive elimination, insertion and deinsertion, electrophilic and nucleophilic attack on ligands carboxylation and decarboxylation and fluxional isomerism.

UNIT – III: Industrial Application of Organometallic Compounds (15 hrs)

Catalytic applications of organometallics: Hydrogenation of olefins, Wacker-Smidt synthesis, oxo process, Repp's catalyst, Monsanto acetic acid process, Zeigler-Natta polymerization of alkenes and oligomerisation, Enantioselective functional group interconversions. Organometallics as protecting and activating groups in organic synthesis. Transmetalation and cyclization reaction of organometallics. Bioorganometallic chemistry and surface organometallic chemistry.

UNIT – IV: Introduction of Bio-inorganic chemistry (10 hrs)

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. Metalloenzymes- Zinc enzymes -carboxypeptidase and Carbonic anhydrase, Vitamin B₁₂, Catalase, Peroxidase, Superoxide dismutase and Copper proteins. Application of Co- ordination compounds in medicinal applications. – Cisplatin – antirheumatoid - gold compound –anti diabetic - anti cancer agents – role of metal ion diagnosis and treatment.

UNIT – V: Transport Proteins

(10 hrs)

Oxygen Carriers – Hemoglobin, myoglobin – structure – function - Oxygenation and stereochemistry – Bohr effect, Non – Heme oxygen carriers – Hemerythrin and Hemocyanin. 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 microorganisms, Nitrogenase enzyme –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, NewAge 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, Bio inorganic chemistry, New Age International private Ltd, reprint 2005.
4. William W. Porterfield, Inorganic Chemistry, An unified approach, academic press inc, 1993.

REFERENCE BOOKS:

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 – Bio inorganic Chemistry, Books & Allied (p) Ltd, first edition, 2004.

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	Unit – 4	4	
	Unit – 5	4	
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	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	1a	
	Unit - 5	1b	

CORE THEORY – 7
CHEMISTRY OF AROMATIC COMPOUNDS AND CONCERTED REACTIONS

SUBJECT CODE: 16PCHC10	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^+ , MnO_2 , TPAP, Moffet, Oppenauer and Swern oxidation of alcohol –oxidative cleavage of Glycols and their related compounds, Oxidative cleavage of Ketones, Aldehydes and Alcohols, Ozonolysis - oxidation of methylene to carbonyl, oxidation of aryl methanes – allylic oxidation of olefins. Reductions: catalytic hydrogenation – Hydrides – Nucleophilic and Electrophilic - MPV reduction- Selectivity in reduction of 4-t-butyl cyclohexanone using selectrides- Synthetic importance of Clemensen 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 homoaromaticity – Hetero aromatic molecules.

UNIT – III: Aromatic Electrophilic, Nucleophilic substitution

(15 hrs)

The arenium ion mechanism. Orientation and reactivity (mono nuclear & poly nuclear aromatic hydrocarbons)-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 tribromobenzene, 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.

Electrophilic substitution of furan, pyrrole, thiophene, pyridine, pyridine N-oxide, quinoline and isoquinoline.

Aromatic Nucleophilic Substitution: Methods for the generation of benzyne intermediate and reactions of aryne 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- Favorskii, Wittig, Neber, Steven, Sommelet- Hauser.

UNIT – V: Pericyclic Reactions

(10 hrs)

Classification –Orbital symmetry – Woodward-Hoffmann rule – FMO analysis of electrocyclic, cycloaddition and sigmatropic reactions –hydrogen shift and carbon shift reactions. Correlation diagram method for cycloaddition reactions ($\pi2s + \pi2s$) and ($\pi4s + \pi2s$) and electrocyclic reactions of butadiene-cyclobutene system and interconversion of hexatriene to cyclohexadiene- Cope and Claisen reactions – 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. Niel Issac, Physical Organic Chemistry, Prentice Hall, second edition, 1996.
5. Jagdambasingh and Jaya Singh, Photochemistry and Pericyclic reaction, New Age International (P) Limited publisher, third edition, 2014.
6. P.S. Kalsi, Organic Reaction and Mechanism, New Age 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.

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

CORE PRACTICAL – 1
ORGANIC CHEMISTRY PRACTICAL – I

SUBJECT CODE: 16PCHC05P	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-benzylbenzoic acid
2. p-Nitrobenzoic acid from p-Nitrotoluene
3. Anthroquinone from anthracene
4. Benzhydrol from benzophenone
5. m-Nitroaniline 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 (any three):*

1. Sym-Tribromobenzene from aniline.
2. p-nitro aniline from acetanilide
3. m-Nitrobenzoic acid from methyl benzoate.
4. 2, 4-Dinitrobenzoic acid from p-nitro toluene.
5. m-Nitro benzoic acid from benzaldehyde
6. p-bromoaniline from acetanilide

III A) 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-Longmana, fourth edition, 2004.

CORE PRACTICAL – II
INORGANIC CHEMISTRY PRACTICAL – I

SUBJECT CODE: 16PCHEC06P	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. Chloropentammine cobalt (III) chloride
8. Bis (acetylacetonato) copper (II)
9. Hexamminenickel (II) chloride
10. Bis (thiocynato) pyridine manganese, (II)

d. Separation of a mixture of two metal ions by paper chromatography. Separation of zinc and magnesium on a cation exchanger.

TEXT BOOKS:

1. A.L. Vogel, Text book of Inorganic quantitative analysis, ELBS, Third edition, 1976.
2. G.S.Vehla, Vogel's textbook 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.

CORE PRACTICAL – III
PHYSICAL CHEMISTRY PRACTICAL-I

SUBJECT CODE: 16PCHEC07P	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 is given. A minimum of 10 – 12 experiments have to be performed.

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-dichlorobenzene, 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 strengths using acid catalysed hydrolysis of methylacetate.
11. Determination of temperature coefficient and energy of activation for the acid catalysed hydrolysis of methylacetate.
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.Ragavan, Practiac physical Chemistry, Published by vivabooks, 2012.
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, NewYork, 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

SUBJECT CODE: 16PCHEE01	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 not required) – 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 **(9 hrs)**

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 Testosterone, Progesterone

UNIT – III: Terpenoids and Carotenoids **(9 hrs)**

Classification, occurrence, general methods of determining structure - isoprene rule. Synthesis of the following molecules – Camphor, Terpeneol, α and β -Carotene, Lycopene.

UNIT – IV: Alkaloids and Anthocyanins **(9 hrs)**

Total synthesis of cocaine, Morphine and Reserpine. Flavones, isoflavones, anthocyanins (Synthesis only)

UNIT – V: Biosynthesis **(9 hrs)**

General principles involved in the biosynthesis of amino acids, alkaloids, steroids and terpenoids. Biosynthesis of Cholesterol, Phenanthrene alkaloid and bile acids.

TEXT BOOKS:

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.

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	Unit – 5	4	
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	Unit – 3	1	1
	Unit – 4	1	
	Unit – 5	1	
Section C	Unit – 1	1	
	Unit – 2	1	
	Unit – 3	1	
	Unit – 4	1a	
	Unit – 5	1b	

SEMESTER - III

**CORE THEORY – 8
SPECTROSCOPY-I**

SUBJECT CODE: 16PCHC11	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 (15 hrs)

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 bands - 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 (10 hrs)

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, Auxochromes, 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 haloketone 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 of with suitable examples.

Applications of UV-VISIBLE spectroscopy to inorganic and organometallic compounds with regard to structural elucidation.

UNIT V: Photoelectron and NQR Spectra

(10 hrs)

Photoelectron spectroscopy – basic principles UPS and XPS – photoelectron spectra- Koopman'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 (OhJay) electron spectroscopy. Determination of Dipole moment, NQR spectroscopy – Theory of NQR – instrumentation – Nuclear quadrupole coupling constants – Applications.

REFERENCE BOOKS:

1. R. S. Drago, Physical Methods for Chemistry, Thomson learning, 1977.
2. Drago R.S, Physical Methods in Chemist, 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. & Chapman G. M. Introduction to Spectroscopy, Books/Cole, fourth edition 2008.
7. Christian G. D. Analytical Chemistry, Wiely, 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 – 3	1	1
	Unit – 4	1	
	Unit – 5	1	
Section C	Unit – 1	1	
	Unit – 2	1a	
	Unit – 3	1b	
	Unit – 4	1	
	Unit - 5	1	

CORE THEORY – 9
SYNTHETIC METHODOLOGY

SUBJECT CODE: 16PCHC12	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 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 R₂LiCu, 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) in organic synthesis. Protection and deprotection of functional groups (-OH, -NH₂, 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-(PPh₃)₃RhCl, lindlar catalyst, 9-BBN, chiral boranes, NaBH₃CN, DIBAL and selectrides - Birch reduction (Hetero cyclic compound). Role of Bu₃SnH, trimethylsilyl 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, Fischer-Indole synthesis, Diels-Alder reaction, Mc-Murry olefination, Prins reaction, Ritter reaction, Mitsunobu reaction, Sharpless asymmetric epoxidation,

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

Retero synthetic analysis 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 in organic synthesis – role of Microwave irradiation and ultrasound waves in organic synthesis – 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 Disconnection 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 retro synthetic analysis vol-2, New central book agencies first reprint, 2008.
13. Michael B. Smith Organic synthesis, McGrawHill, (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:

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Section A	Unit – 1	4	
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	Unit – 3	4	
	Unit – 4	4	
	Unit – 5	4	
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	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	1a	
	Unit - 5	1b	

CORE THEORY – 10
THERMODYNAMICS AND ELECTROCHEMISTRY

SUBJECT CODE: 16PCHC13	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 electrochemistry.

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- Plancks radiation law – electron in metals.

UNIT – IV: Electrochemistry of Solutions

(15 hrs)

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.

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 Electrochemistry

(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. Mechanism of electrode reaction- The Butler-Volmer equation for one step and multistep electron transfer reactions- significance of exchange current density and symmetry factor. Polarization and over potential-A brief account of hydrogen overpotential- factors affecting. Hydrogen over potential-mechanism of Hydrogen evolution and oxygen evolution-concentration polarization.

Corrosion: Theories of corrosion-Techniques of inhibiting corrosion-Pourbaix diagram- Evans diagram-Electro deposition –principles and applications. Fuel cells: Construction and principles of operation and applications

TEXT BOOKS:

1. J.O. M. Bokris and A.K.N. Reddy, Electrochemistry, Vol 1&2, Kluwer academic/Plenum publishers, New York, Second edition.2002.
2. S. Glasstone Introduction to Electrochemistry, Liton educational Publishing INC, reprint2010.
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 McClellan and Statistical thermodynamics, Chapman and Hall, London.1973.
6. Nester Perez, Electro chemistry 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	
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	Unit – 2	1	
	Unit – 3	1	1
	Unit – 4	1	
	Unit – 5	1	
Section C	Unit – 1	1	
	Unit – 2	1a	
	Unit – 3	1b	
	Unit – 4	1	
	Unit - 5	1	

ELECTIVE – II
SOLID STATE AND NANO CHEMISTRY

SUBJECT CODE: 16PCHEE03	THEORY	MARKS 100
SEMESTER: III	CREDITS: 3	TOTAL HOURS: 60

COURSE OBJECTIVES:

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

UNIT - I: Solid state Chemistry

(15 hrs)

Classification of crystals and elements of symmetry (including glide planes and screw axis) Bravais lattices; planes and indices, X-ray diffraction and Bragg's law, powder diffraction-refinement and structure solution of some compounds. 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, crystalite, 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 & imperfect crystals, lattice Defects - types of defects. Order & 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) Reactions of solid state and 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, paramagnetism – X. Langevin's theory & paramagnetic susceptibility of solids. Temperature independent paramagnetism - spin cross over phenomena. Simplification of Van Vleck equation and magnitude of magnetic moments. Determination of magnetic susceptibility by Gouy and Faraday method.

Domain theory – Hysterisis Loop – Applications. Properties of Spinel, Ilmenites, Perovskite and Magneto-plumbites. Hard and Soft magnetic materials. Superconductors – superconductivity in metals, alloys and ceramics materials (mixed oxides) BCS theory, Meissner effect, type I & II superconductors, application Fullerenes as superconductors.

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

Carbon based nanomaterials, Metal based materials, dendrimers and composites. Classification of Nanomaterials based on dimensions. Properties of nano materials -Size dependent properties - Mechanical, Physical and Chemical properties. Quantum effects. Synthesis of nano materials - Bottom up and top down methods. Characterization methods of nano materials – XRD - Debye Scherrer method, Scanning electron microscopy (SEM) -morphology, atomic Force microscopy (AFM), Transition Electron Microscopy (TEM) -Crystallite size and SAED pattern.

UNIT - V: Application of Nanomaterials (10 hrs)

Energy-fuel cells, Microbial fuel cell, hydrogen storage, nanophosphors 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, Nanocoatings and paintings. Cosmetic applications. Disadvantages of Nanomaterials –Nanotoxicity, Green Nanochemistry.

REFERENCE BOOKS:

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, Weinheim, 2004.
6. Kenneth J. Klabunde (Eds), Nanoscale Materials Science, John Wiley & Sons, Inc., 2001.
7. C.S.S.R. Kumar, J. Hormes, C. Leuschner, Nanofabrication towards biomedical applications, Wiley –VCH Verlag GmbH & Co, Weinheim, 2004.
8. W. Rainer, Nano Electronics and information Technology, Wiley, 2003.

9. K.E. Drexler, Nano systems, Wiley, 1992.
10. G.Cao, Nanostructures and Nanomaterials: Synthesis, properties and applications, Imperial College Press, 2004.

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

SEMESTER - IV

**CORE THEORY – 11
PHOTOCHEMISTRY**

SUBJECT CODE: 16PCHC15	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: Organic Photochemistry

(10 hrs)

Photo chemistry of ketones – Norrish Type-I, Norrish type –II - Photo reduction, - photo chemistry of olefins - cis –trans isomerisation - Photocycloaddition, - Paterno –Buchi reaction – photo chemistry of aromatic compounds – photo rearrangements - Di- π methane rearrangement, Barton reaction and Photo fries reaction – Photochemistry of cyclohexadienones – photo chemistry of santonin - synthesis of Vitamin D.

UNIT – IV: Photochemistry of Co-ordination Compounds

(10 hrs)

Types of Photochemical 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 electro chemistry- Role of Ruthenium bi pyridine

[Ru(bpy)₃] complexes in solar energy conversion- photosynthesis.

UNIT – V: Applied Photochemistry

(15 hrs)

The solar spectrum, antennas, reaction centers, photoprocesses in organic, inorganic, and sensitized solar cells. Excitons, polarons, solitons, semiconductor junctions, photocurrent and photovoltage, Photocatalysis, photodamage and repair, DNA photodynamic 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, Londaon,1989.
3. J. C. Scaiano, ed., "CRC Handbook of Organic Photochemistry", vol. 1 and 2, CRC Press,Boca Raton, Florida, 1989.

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

CORE THEORY – 12
SPECTROSCOPY-II

SUBJECT CODE: 16PCHC16	THEORY	MARKS 100
SEMESTER: IV	CREDITS: 4	TOTAL HOURS: 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 ^{13}C - 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. ^{13}C - NMR applications to structure elucidation of simple organic molecules – complete decoupled ^{13}C NMR – off resonance spectra- chemical shift values. Elementary treatment of two- dimensional NMR spectroscopy, NOESY, COSY, and DEPT.

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

Applications of ^{31}P , ^{19}F , ^{119}Sn and ^{195}Pt NMR spectroscopy in the structural assessment of simple inorganic compounds. Inter and intramolecular exchange studies using NMR. Applications of NMR in the study of co-ordination 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 Fe⁵⁷, Sn¹¹⁹ and I¹²⁹ 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, McLafferty 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, TataMcGraw-Hill, New Delhi, fourth edition, 2010.
2. D. A. McQuarrie and J.D. Simon –Physical Chemistry, Molecular approach Viva studentsEd, 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. Craddock, Structural Methods in Inorganic Chemist 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, ¹³C 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 Pbulishers, 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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CORE PRACTICAL – 4
ELECTRO ANALYTICAL PRACTICAL

SUBJECT CODE: 16PCHC14P	PRACTICAL	MARKS 100
SEMESTER: IV	CREDITS: 4	TOTAL HOURS: 60

COURSE OBJECTIVES:

- To help the students to understand and apply the concepts of electroanalytical 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.Ragavan, Practiacal physical Chemistry, Published by viva books, 2012.
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 PRACTICAL – I
ANALYTICAL CHEMISTRY PRACTICAL

SUBJECT CODE: 16PCHEE02P	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 (ANY FOUR):

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of glucose (Bertrands Methods)
4. Saponification of fat or oil.
5. Iodine value of an oil.
6. Estimation of Ketone.

B. SPECTRAL INTERPRETATION OF ORGANIC COMPOUNDS. UV, IR, PMR AND MASS SPECTRA OF 15 COMPOUNDS.

1. 1, 3, 5-Trimethylbenzene
2. Pinacolone
3. propyl amine
4. p-Methoxybenzyl alcohol
5. Benzyl bromide
6. Phenyl acetone
7. 2-Methoxyethyl acetate
8. Acetone
9. Isopropyl alcohol
10. Acetaldehyde diacetate
11. 2-N, N-Dimethylamino ethanol
12. Pyridine
13. 4-Picoline
14. 1, 3 dibromo-1, 1-dichloropropene
15. Cinnamaldehyde

C. SPECTRAL INTERPRETATION OF INORGANIC COMPOUNDS

1. ^{31}P NMR Spectra of methylphosphate
2. ^{31}P NMR Spectra of HPF_2
3. ^{19}F NMR Spectra of ClF_3
4. ^1H NMR Spectra of Tris (ethylthioacetato) cobalt (III)
5. Expanded high resolution NMR spectra of (N-propylisonitrosoacetylacetonato) (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 nitropentamminecobalt (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 $[\text{Fe}(\text{CN})_6]^{3-}$
17. Mossbauer spectra $[\text{Fe}(\text{CN})_6]^{4-}$

D. QUANTITATIVE ANALYSIS OF COMPLEX MATERIALS

To impart the techniques of analysis of ores, alloys and preparation the analysis inorganic complex compounds. (For Internal Assessments Only)

a) Analysis of Ores:

1. Determination of percentage of calcium and magnesium in dolomite.
2. Determination of percentage of MnO_2 in pyrolusite.

b) Analysis of Alloys:

1. Estimation of tin and lead in solder.
2. Estimation of copper and zinc in brass.
3. Estimation of chromium and nickel in stainless steel.

c) Analysis of Inorganic Complex Compounds:

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

d) Instrumental methods

1. Analysis of Ni and Cr in stainless steel alloy by spectrophotometry.
2. Estimation of calcium present in calcium lactate tablets by spectrophotometry.

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