

M.Sc., CHEMISTRY (2017 – 2018)

Sl. No	SEM	Category	Paper Code	Title of the Paper	Maximum Marks			Minimum Marks			Hours Week	Credits
					CIA	E.E.	Total	CIA	E.E	Total		
1	I	Core	17P1CHC1	Physical Chemistry – I	25	75	100	10	30	50	7	5
2		Core	17P1CHC2	Inorganic Chemistry – I	25	75	100	10	30	50	6	4
3		Core	17P1CHC3	Analytical chemistry	25	75	100	10	30	50	6	5
4		Core	17P1CHCP1	Physical Chemistry Practical – I (non Electrical)	40	60	100	16	24	50	6	3
5		Major Elective-I	17P1CHEL1A 17P1CHEL1B	Medicinal Chemistry/ Bio Chemistry	25	75	100	10	30	50	5	4
6	II	Core	17P2CHC4	Organic Chemistry – I	25	75	100	10	30	50	5	5
7		Core	17P2CHC5	Physical Chemistry – II	25	75	100	10	30	50	5	5
8		Core	17P2CHC6	Physical Methods in Chemistry - I	25	75	100	10	30	50	5	5
9		Core	17P2CHC7	Polymer Chemistry	25	75	100	10	30	50	5	4
10		Core	17P2CHCP2	Physical Chemistry Practical-II (Electrical)	40	60	100	16	24	50	5	3
11		Major Elective-II	17P2CHEL2A 17P2CHEL2B	Paint Chemistry / Cheminformatics	25	75	100	10	30	50	5	4
12	III	Core	17P3CHC8	Organic Chemistry – II	25	75	100	10	30	50	5	5
13		Core	17P3CHC9	Physical Methods in Chemistry-II	25	75	100	10	30	50	5	5
14		Core	17P3CHC10	Industrial Chemistry	25	75	100	10	30	50	5	5
15		Core	17P3CHCP3	Organic Practical – I	40	60	100	16	24	50	5	3
16		Core	17P3CHCP4	Organic Practical – II	40	60	100	16	24	50	5	3
17		EDC	17P3CHEDC	Chemistry in Every Day life	25	75	100	10	30	50	4	-
				Communicative skill & Personality development	-	-	-	-	-	-	1	-
18	IV	Core	17P4CHC11	Inorganic Chemistry – II	25	75	100	10	30	50	6	6
19		Core	17P4CHCP5	Inorganic Practical – I	40	60	100	16	24	50	6	3
20		Core	17P4CHCP6	Inorganic Practical – II	40	60	100	16	24	50	6	3
21		Major Elective-III	17P4CHEL3A/ 17P4CHEL3B	Recent Trends in Chemistry / Applied Chemistry	25	75	100	10	30	50	6	4
22		CN	17P4CHCN	Comprehensive Knowledge Test	-	100	100	-	50	50	5	2
23		Project	17P4CHPR	Project Industrial internship (Along with Industrial visit)	40	60	100	16	24	50	-	4
				Communicative skill and personality development	-	-	-	-	-	-	1	-
			Total			2300				120	90	

M.Sc., CHEMISTRY (2017 – 2018)

Paper Code	Total No. Of Papers	Total Marks	Total Credits	Classification
Core	17	1700	72	✓
Elective	3	300	12	✓
E.D.C	1	100	---	✓
Project	1	100	4	x
Comprehension	1	100	2	✓
Soft skill using Language lab	--	--	---	X
Total	23	2300	90	

**A.VEERIYA VANDAYAR MEMORIAL SRI PUSHPAM COLLEGE
(AUTONOMOUS),
POONDI, THANJAVUR DIST.**

**Question Pattern for UG and PG Programmes for students to
be admitted during 2017 – 2018 and afterwards**

Total Marks: 75

QUESTION PATTERN

**SECTION – A
(Question 1 to 10)**

10 x 2 = 20 Marks

1. Short Answer Questions
2. Two Questions from each units (All are answerable)

**SECTION – B
(Question 11 to 15)**

5 x 5 = 25 Marks

1. 5 Paragraph type questions with "either / or" type choice.
2. One question from each unit of the Syllabus.
3. Answer all the questions.

**SECTION – C
(Question 16 to 20)**

3 x 10 = 30 Marks

1. 5 Essay type questions – any three are answerable.
2. One questions from each unit of the Syllabus.

Semester	Subject Code	Title of the Paper	Hours of Teaching/Week	No. of Credits
I	17P1CHC1	Physical Chemistry – I	7	5

UNIT – I Group theory

Principles – Elements of group theory –properties of a group and subgroup- classes- group multiplication tables – symmetry elements and operations – inter relations among symmetry operation point groups of molecules - Matrix representations theory- reducible and irreducible representations – Great orthogonality theorem and its consequences –construction of character tables (C_{2v} , C_{3v})

Applications of group theory:- Evaluation of energies and MO's for system like ethylene, butadiene and benzene- hybridization concepts- CH_4 and BF_3 only. Finding symmetry of normal and active modes of vibration for H_2O and BF_3 only. Symmetry selection rules for IR and Raman Spectra.

UNIT – II

Quantum Chemistry – I

Inadequacy of classical mechanics, Black body radiation, Planck's quantum concepts, Photoelectric effect. Bohr's theory of hydrogen atom: Hydrogen spectra, wave –particle dualism, Uncertainty principle, Inadequacy of old quantum theory.

Schrodinger wave equation, Derivation of time dependent Schrodinger - Postulates of quantum mechanics, Operator algebra: operator, linear and Hermitian, Verification of operators Hamiltonian - Eigen functions and Eigen values, angular momentum operator, commutative relations and related theorems.

Applications of wave mechanics to simple systems – particle in a box, one and three – dimensional, distortion of the box and John –Teller effect, quantum numbers, zero – point energy, orthogonality and normalisation, finite potential barrier – tunneling.

UNIT – III

Chemical Kinetics – I Theories of reaction rates – Absolute reaction rate theory Collision theory – Steric effect – limitations potential energy surface, Transmission coefficient - ARR theory – thermodynamic treatment – relation with Arrhenius equation Hinshelwood theory, ARR theory – Significance of reaction co- ordinate –Kinetic isotope effect – Marcus theory of electron transfer processes.

Principle of microscopic reversibility – Steady – state approximation - any three examples specify– Chain reactions. Thermal and photochemical reactions between hydrogen and halogens – Explosions and hydrogen – oxygen reactions.

UNIT – IV

Molecular Thermodynamics – Calculation of thermodynamic probability of a system – difference between thermodynamic probability and statistical probability – Phase space – Microstate and macro state – methods of determination - derivation of Boltzmann distribution equation – physical significance of partition function – translational, rotational vibrational and electronic partition function.

Relationship between partition function and thermodynamic properties such as E, H, CP, CV, P. Derivation of $PV=RT$ molecular interpretation of entropy – derivation of $S=k \ln w$ Sackur Tetrode equation-Calculation of S, A, G etc from partition functions – calculation of equilibrium constants for very simple reactions.

UNIT – V

Fast reaction Techniques: Introduction, flow methods (Continuous and stopped flow techniques) – Relaxation methods (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, Shock tube method) – Molecular beam method.

Photochemistry: Basic principles of Photochemistry-Jablonski diagram (Quenching) – Stern – Volmer equation and its applications – experimental techniques in photochemistry chemical actinometers – laser and their applications.

Radiation Chemistry: Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – Definition of G value – Curie – Linear energy transfer LET and Rad Scavenging techniques – use of dosimeter and dosimeters in radiation chemistry- applications of radiation chemistry.

Reference:-

1. Albert Cotton, Chemical Applications of Group Theory, Third Edition John Wiley & Singapore 2003.
2. Robert L. Carter, Molecular Symmetry and Group Theory John Wiley and Sons. Inc. New York, 1998.
3. R.L. Flurry, Jr. Symmetry Groups – Prentice Hall, New Jersey 1980.
4. B.E. Douglas and C.A. Hollingsworth, Symmetry in Bonding and Spectra – An Introduction Academic Press New York, 1985.
5. R.K. Prasad, Quantum chemistry
6. A.K. Chandra, Introduction Quantum Chemistry 4th ed., Tata McGraw Hill 1984.
7. Doggett & Sutcliffe, Mathematics for Chemists, Longman Scientific & Technical New York, USA, 1995.
8. D.A. McQuarrie, Quantum Chemistry, University Science Books, 1998. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill, 1968.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
I	17P1CHC2	Inorganic Chemistry – I	6	4

UNIT – I

Acids and Bases: Bronsted and Lewis acids and bases pH, pKa, acid – base concept in non aqueous medium buffer solution, Protonic Acids – Proton Affinities – Differentiating and leveling solvents – Acidic-Behaviour of the Binary hydrides – strength of oxyacids – Hydrolysis – Amphoteric oxides – Non protonic concepts of acid – Base Reactions – Lux concept –Solvent ion theory of Acids and Bases – Liquid Ammonia, Acetic acid, bromine trifluoride, Dinitrogen tetroxide, liquid hydrogen fluoride as solvents – classification on Acids and Bases as Hard or Soft – Acid-Base strength and Hardness and softness –Theoretical basis of Hardness and softness – Electro negativity and Hardness and Softness.

UNIT – II

Nuclear Chemistry: Radioactive decay – Theories of decay processes – Laws of radioactivity – Detection and Measurements of radiations – Nuclear structure – Composition of nuclei – properties of nuclei – nuclear radii – nuclear spin etc. nuclear stability – nuclear models – liquid drop, shell and collective models – Nuclear forces – meson field theory.

Artificial Radioactivity: Nuclear reactions – transmutation – Stripping and pick up, Fission products and fission yields, fusion, spallation and fragmentation reactions scattering reactions – nuclear cross section–Q–value Nuclear reactors – charged particle accelerators – neutron sources –gamma ray and X – ray sources . Radioactive techniques – tracer technique neutron activation and isotopic dilution analysis, counting techniques such as G.M. ionization and proportional counter. Applications of nuclear science in agriculture and biology. Radiation risks and medical benefits – Natural and manmade isotopes.

UNIT – III

Polyacid anions: Basic building units of vanadate, molybdate, and tungstate ions – apex sharong (structure only) Heteropoly anions – structure only Rings Phosphazenes – structure – Boron hydrides and carboranes

Clusters: Metal cluster – dinuclear – structures of $\text{Re}_2\text{Cl}_8^{2-}$ qualitative M.O. diagrams for dinuclear rhenium and molybdenum complexes to explain the strength of quadrupole bond – Cluster bonding models – Wade and Lohar.

UNIT – I V

Solid state chemistry: Crystal structure – classification of ionic structure – Ax_1 , Ax_2 , Ax_3 types – Ax type (Zns, NaCl, CsCl) structure only – AX_2 type (fluorite, rutile, beto crystalalite) structure only – layer structure – CdI_2 , nickel arsenate. schottky and frenkel defects – explanation and calculation of number of defects per cm – metal excess defect – F-centre and interstitial ions – metal deficiency defects – positive ion absent – extra interstitial negative ions.

UNIT – V

Main Group Chemistry: Chemistry of boron – borane higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes, silicon nitrides, siloxanes and silicates. P-N compounds, cyclophosphazenes S.N. compounds – S_4 N_4 (SN). **Ionic Model:** Lattice energy – Born – Lande equation – born haber cycle-radius ratio-fajans rule-Kapustinski equation – High Tc superconductors – Solid state reactions – Types and examples.

References:

1. Badie E. Douglas and Danl H. McDaniel Concepts and models in Inorganic Chemistry, Indian Edition, 1970, Oxford and IBH Publishing Co., New Delhi.
2. J.D. Lee. A New concise Inorganic Chemistry, 4th Edition, ELBS, 1995 (UNIT - II)
3. G. Friedlander, J.W. Kennedy and J.M. Miller, Nuclear and Radiochemistry (Unit-III)
4. Keith F.P Purchell and John C. Kotz, Inorganic Chemistry, Saunders Golden Sunburst series, W.B. Saunders company, Philadelphia.
5. Cotton and Wilkinson, Advanced Inorganic Chemistry, 5th Edition, John Wiley & sons, New York (Unit IV)
6. W.Kain and B. Schwederski, Bioinorganic Chemistry of life, John Wiley and Sons, New York (Unit V)
7. James E. Huheey, Ellen A. Keiter and Richard L. Richard L. Keiter, Inorganic Chemistry Principles of structure and Reactivity, 4th Edition, Addition -Wesley, New York (Unit - I)
8. Shriver and Atkins, Inorganic Chemistry, III Edition Oxford, 1999, India Gopsons Pvt. Ltd., A - 14 Sector Noida.
9. Advanced Inorganic Chemistry - Gurdeep Raj - 23rd revised and enlarged edition - Goal Publishing House, Meerut.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
I	17P1CHC3	Analytical Chemistry	6	5

UNIT I

Data and Error Analysis:

Various types of Error – Accuracy, precision, significant figures – Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – Describing data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements – Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, Paired t-Test – Analysis of variance (ANOVA) – Correlation and Regression – Curve fitting , Fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – General polynomial equation fitting, linearizing transformations, exponential function fit – r and its abuse – multiple linear regression analysis, elementary aspects.

UNIT II

Chromatography:

Principles of ion exchange, paper, thin layer and column Chromatography techniques – Columns, adsorbents, methods, R_f values, McReynold's constants and their uses – HPTLC, HPLC techniques – Adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques: methods, principles and uses.

UNIT III

Thermo analytical methods: Principles, instrumentation and applications of Thermogravimetry Analysis (TGA) – Differential Thermal Analysis (DTA) – differences between TGA and DTA - Differential Scanning Calorimetry (DSC). Thermometric titrations.

Photoelectron Spectroscopy – Principles – Auger electron spectroscopy – Electron Spectra for Chemical Analysis (ESCA).

UNIT IV

Atomic Absorption Spectroscopy : Principle – difference between AAS & FES, theory – instrumentation – hollow cathode lamp- burners- oxidants – fuels – interference and applications – Flame Emission Spectroscopy – Principles – instrumentation – interference – limitations of FES – factors that influence the intensity of Emitted radiations – applications – Standard addition and internal standard methods.

UNIT V

Voltametry: Principles – polarography – principles and introduction instruments current voltage- relationship polarographic waves – equation – half wave potential-reversible and irreversible waves- residual current – migration current – polarographic cells- dropping mercury electrode – advantages of DME – aqua salt bridge- saturated calomel electrode – applications- qualitative and quantitative analysis – inorganic and organic polarography. Tensametry- chloro potentiometry- instrumentation and applications- Cyclic and stripping Voltametry- principles and applications

References:

1. D.B.Hibbert and J.J. Gooding, Data Analysis for chemistry, Oxford University Press, 2006
2. J.Topping, Errors of Observation and their treatment, Fourth Edn., Chapman Hall, London, 1984
3. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall, New York.
4. V.K.Srivastava & K.K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2nd ed, 1981.
5. Willard, Merrit, Dean and Settle, Instrumental methods of Analysis CBS Publishers and Distributors, 6th ed 1986.
6. Skoog, D. A., West, D. M., Holler, F. J., Fundamentals of Analytical Chemistry, 7th edition, Harcourt College Publishers, Singapore. (Pages 523 - 665).
7. A.Sharma, S.G. Schulman, Introduction to Fluorescence Spectroscopy, Wiley-Interscience. New York, 1999
8. C.N.Banwell and E.M.McCash, Fundamentals of Molecular spectroscopy, 4th ed., Tata McGraw-Hill, New Delhi, 1994.
9. Vogel, A. I., Text book of Quantitative Inorganic Analysis, ELBS.
10. Daniel C Harris, Quantitative Chemical Analysis, 4th ed., W. H. Freeman and Company, New York, 1995.
11. S.C.Gupta, Fundamentals of Statistics, 6th ed., Himalaya Publ. House, Delhi, 2006.
12. B.K. Sharma, Instrumental methods of Chemical analysis, Himalaya Publ. House, Delhi, 2006.
13. Gurdeep Chatwal, Instrumental methods of Chemical analysis,

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching/Week	No. of Credits
I	17P1CHCP1	Physical Chemistry Practical-I (non Electrical)	6	3

Non –Electricals

1. Determination of CST and study of the effect of impurity on CST
2. Determination of distribution coefficient and determination of equilibrium Constant for the formation of KI_3
3. Determination of the rate constant for Persulphate oxidation both by titrimetry and Colorimetry.
4. Comparison of acid strengths by Kinetics.
5. Determination of the energy of activation and frequency factor.
6. Association factor of benzoic acid between benzene and water
7. Determination of molecular weight by Rast macro method
8. Phase diagram – simple eutectic system
9. Phase diagram – three component system
10. Adsorption of oxalic acid on charcoal.
11. Determination of molecular weight by Transition Temperature Method

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credit
I	17P1CHEL1A	Major Elective-I Medicinal Chemistry	5	4

UNIT – I

Definitions: The nature and source of drugs, pharmacologically active principles in plants. The terms- Drugs, pharmacology, pharmacognosy, pharmacy, Therapeutics, Toxicology, chemotherapy, pharmacopoeia, First aid –Important rules of first aid - Cuts, Abrasions and Bruises, Fractures, bleeding for blood, maintain breathing. Burns and fainting. First aid box -T.B, Asthma, Jaundice, Piles, Leprosy, Typhoid, Malaria, Cholera, Filariasis - causes- symptoms-diagnosis –prevention and treatment.

Unit II

Anticonvulsants, Stimulants and Antipyretic Analgesics

Anticonvulsants - classification, synthesis and mode of action; Muscle relaxants-classification, synthesis and mode of action. Central nervous system stimulants-classification, synthesis and mode of action; Antipyretic analgesics classification, synthesis and mode of action;

Unit III

Antihistamines, Anti-inflammatory and Antiparkinson drugs

Antihistaminics - synthesis and mode of action of histamine H1 receptor antagonists and histamine H2-receptor blockers; prevention of histamine release; structure-activity relationships amongst H1-receptor blockers. Non-steroidal anti-inflammatory drugs(NSAID)-synthesis and mode of action of heteroarylacetic acid analogues, arylacetic acid analogues, arylpropionic acid analogues, naphthalene acetic acid analogues, gold compounds, salicylic acid analogues and pyrazolones and pyrazolodiones; Antiparkinsonism agents-synthesis and mode of action of piperidine analogues, pyrrolidine analogues and phenothiazine analogues.

UNIT – IV

Anaesthetics: Ideal anaesthetic agent – classification according to mode of action, General Anaesthetics – volatile ether, vinyl ether, Halothane, Trichloro ethylene – structure, advantages and disadvantages, non-volatile – Thiopental sodium – properties structure, advantages and disadvantages , local anaesthetics- requisites, cocaine-structure and advantages antiseptics and disinfectants – distinction between disinfectants and antiseptics, phenol co-efficient. Psychedelic drugs- lysergic acid diethylamide (LSD)- Pharmacological action of LSD- mechanism of action – therapeutic uses – adverse effects. Marijuana – Pharmacological action and therapeutic uses.

UNIT – V

Cancer- types causes spread treatment – antineoplastic drugs- alkylating agents, antimetabolise, hormones, antibiotics, radioactive isotopes, adrenocorticosteroids. **Diabetes** –types- control of diabetes insulin, oral hypoglycaemic sulphonyl ureas-tolbutamide, chlorpropamide glibenclamide-structure and uses. Biguanides – phenformin and metformin. **AIDS** – Causes – symptoms – prevention and treatment.

Text Books:-

1. Jaya Shree ghosh – A textbook of pharmaceutical chemistry.
2. Ashutosh Kar, **Medicinal Chemistry**, New Age International, 1996.
3. W.O.Foye, **Principles of medicinal chemistry**, 2nd Edn., Lea & Febiger, Philadelphia, 1981.

Reference Books:-

1. M.E.Wolff, **Burger's medicinal chemistry**, 4th Edn., John Wiley & Sons, New York, 1981.
2. F.F.Blicke and R.H.Cox, **Medicinal Chemistry**, John Wiley & Sons, New York, 1959.
3. D.Lednicer and L.A.Mitscher, **Organic Chemistry of drug synthesis**, John Wiley & Sons, New York, 1959.
4. E.Hoover, **Remington's Pharmaceutical sciences**, 15th Edn. Mack Publ.Company, Easton, 1975.
5. S. Lakshmi – pharmaceutical chemistry.
6. K.Bhawate Sundari – Applied chemistry.

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credits
I	17P1CHEL1B	Major Elective-I Spectroscopy	5	4

UNIT – I

U.V. Spectroscopy – Basic principles of electronic transitions – solvent effects – woodwards – fisher rules Differentiation of cis & trans isomers, ORD & CD Theory –Axial haloketon rule – Octant Rule Comparison between ORD & CD X- Ray – Photo Electron spectroscopy –Theory – instrumentation – application – types – AES – ESCA – applications.

UNIT – II

IR & Raman Spectroscopy – Principles - instrumentation – applications – structure elucidation – vibrational spectra Harmonic and unharmonic oscillators – vibrational spectra of diatomic molecule and polyatomic molecules – Fourier transform IR – vibrational spectra of carbonyl compounds. Finger print region – identification of functional groups – H – bonding – Factors influencing vibrational frequency – Raman Spectroscopy – Principles – polarization of light and Raman effect – comparison of IR & Raman for simple molecules – combined uses of IR & Raman spectroscopy in the structural elucidation of molecules like CIF_3 NO_3 CIO_3

UNIT – III

Nuclear Magnetic Resonance Spectroscopy: Nuclear Magnetic resonance spectroscopy – chemical and magnetic non – equivalency – coupling constant First and Non First order spectra – Dependence of J on dehydral angle – Karplus equation – Double Resonance shift reagent – NOE, Decoupling of protons, off resonance. C^{13} - NMR - Basic principles – FT NMR – Importance of NOE and applications.

UNIT – IV

Mossbauer Spectroscopy: Mossbauer transition – Doppler effect Isomer shift – quadrupole splitting. Magnetic field effect – Application to iron and tin compounds NQR : Theory Instrumentation – application . Mass spectroscopy: Base peak – isotopic peak – metastable peak – Nitrogen rule – McLafferty rearrangement, Ring rule – CI FI and FAB technique – GC /MS Application.

UNIT – V

Application of IR, UV, NMR and Mass spectroscopy in the structural elucidation of organic compounds (Minimum 25 problems worked out) ESR : Factors affecting “g” value – Hyperfine splitting – Kramer degeneracy – zero field splitting . Application to organic and inorganic compounds – CIDNP – Technique.

Reference:

1. William kemp, Organic spectroscopy
2. Sharma, Y.R. Absorption spectroscopy of organic molecules.
3. Sylverstein and Basler and Morril, Spectral identification of organic compounds.
4. Jagmohan, organic spectroscopy, principles.
5. Dash A.N. Analytical chemistry
6. Vogal A.I. Text book of quantitative inorganic Analysis.
7. Sharma B.L. Spectroscopy
8. Sharma B.K. Instrumental methods of Chemical Analysis
9. Kalsi P.S. Organic spectroscopy. New agri international
10. Drago. R.S. Physical methods in chemistry
11. Ebsworth, structural Inorganic Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
II	17P2CHC4	Organic Chemistry – I	5	5

UNIT – I Nomenclature ,Heterocyclics and Natural Products

Nomenclature of alicyclic, bicyclic, tricyclic compounds (Basic skeletal structures only with or without one substituent) and heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur

Heterocyclics: synthesis and reactivity of the following heterocyclics – pyrazoles, oxazole, imadazole, thiazole, pyridazines and pyrazines. (synthesis of simple alkyl and aryl substituted derivatives are also expected)

Steroids: Conversion of cholesterol into progesterone and Testosterone. Stereochemistry and structure elucidation of cholesterol (by chemical degradation)

UNIT II Aromaticity

Aromatic character: Five - Six, seven-, and eight-membered rings - Other systems with aromatic sextets - Huckel's theory of aromaticity, Concept of homo aromaticity and anti aromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and anti aromaticity, systems with 2,4,8,10 electrons and more than 10 electrons, alternant and non-alternant hydrocarbons. Bonding properties of systems. Heteroaromatic molecules. Annulenes, sydnones and fullerenes.

UNIT- III Stereochemistry :

Optical activity and criteria for chirality - Enantiotopic, diastereotopic and Prochiral centres. Projection formulae and inter conversions. Absolute configuration - sequence rule - molecules with more than one chiral centre, alicyclic compounds, pseudo asymmetric center - RS notation for alicyclic compounds.

Stereo selective and stereo specific reactions - Asymmetric synthesis and its principle - Cram's rule. Conformations of di-substituted cyclohexanes and decalins

Dynamic Stereochemistry

Winstein-Eliel equation-curtin-Hammett principle. Conformation, Reactivity and mechanism of cyclic systems - esterification of an alcohol, chromic acid oxidation of cyclohexanol. De amination of 2-amino cyclohexanol.

UNIT IV Nucleophilic Substitution

Aliphatic nucleophilic substitution: S_N1 , S_N2 , S_Ni mechanism - effect of substrate, structure, leaving group, attacking nucleophile and solvent - neighbouring group participation - substitution at allylic carbons and reactivity, ambident nucleophiles - alkylation and acylation of amines, von Braun reaction - hydrolysis of esters.

Aromatic nucleophilic substitution: S_NAr , S_N1 and benzyne Mechanism - effect of substrate structure leaving group, attacking nucleophile and solvent. Zeigler alkylation, Chichibabin reaction - reaction involving diazonium ion, cine substitution, Von Richter reaction.

UNIT V Organic Photochemistry

Organic Photochemistry - Fundamental concepts - Jablonski diagram - Energy transfer, characteristics of photoreactions, photo reduction and photo oxidation, photoreactions of ketones and **enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds** Photolytic cycloadditions and photolytic rearrangements - Photosensitization - Photoadditions - Barton reaction - Paterno Buchi reaction.

References

1. J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and structure*, 5th ed. Wiley, 2000
2. D. Nasipuri, *Stereochemistry of organic compounds-Principles and applications*, New Age International, 2nd Edition, 2002.
3. I.L. Finar, *Organic Chemistry*, Vol.II, 5th ed., ELBS 1975
4. R.K. Bansal, *Organic Reaction Mechanisms*, Tata McGraw Hill, 1975.
5. R.T. Morrison and R.N. Boyd, *Organic Chemistry*, 6th ed., Pearson, 1992
6. J.D. Coyle, *Organic Photochemistry - Wiley*, 1985.
7. J.M. Coxon, B. Halton, *Organic Photochemistry*, Camb. Uni. Press, 2nd edition, 1987.
8. G.R. Chatwal, *Organic Photochemistry*, Himalaya Publications house, 1st edition, 1998.
9. P.S. Kalsi, *Stereochemistry*, Wiley eastern limited, New Delhi, 1990
10. V.K.Ahluwalia and R.K.Parashar, *Organic reaction mechanisms*
11. S.M.Mukherji and S.P.Singh, *Reaction mechanism in organic chemistry*.
12. Bhupinder Mehta and Manju Mehta "Organic Chemistry", PHI Learning Pvt Ltd, New Delhi – 110001.(2012).

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credits
II	17P2CHC5	Physical Chemistry - II	5	5

UNIT - I

Quantum Chemistry – II

Rigid rotator – harmonic oscillator – rotational and vibrational quantum numbers and selection rules for rotational and vibrational transitions – Bohr’s correspondence principle – hydrogen atom – shapes and nodal properties of orbital. Principles of approximation methods – many electron atoms – wave functions – one electron orbital – Pauli’s principles and / Slater determinants – variation methods application to hydrogen and helium atoms – perturbation method for non degenerate systems – application of perturbation theory to helium atom. Hartree – Folk self consistent field method – L.S. and J-J coupling. Born – Oppenheimer approximation Huckel pi – election theory and its application to ethylene, butadiene and benzene.

UNIT – II

Quantum Statistics

Quantum statistics – Bose Einstein and Fermi – Dirac statistics – Comparison of them with MB. Statistics – application of B.E. statistics of photon gas and super fluidity of liquid helium. Application of F.D. statistics to electron gas and thermionic emission. Heat capacity of solids – Einstein and Debye’s treatment – Concepts of negative Kelvin temperature.

Third law of Thermodynamics:

Law of Thermodynamics: Need for the third law – Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities as absolute zero – statistical meaning of third law – apparent exception to the third law.

Non – equilibrium Thermodynamics: Thermodynamics of irreversible processes – Onsager reciprocal relations – steady state conditions.

UNIT – III

Ionics

Transport of ions in solution – Debye – Huckel Onsager theory – Debye – Falkenhagen and wein effects – Modification to Debye – Huckel Onsager theory – Activity of ions in solutions – Experimental determinations – Debye – Huckel limiting law. Activity coefficient at higher concentration – Bejrum model. Electrode – electrolyte equilibrium – Nernst equation and its limitations – equilibrium electrode potential – Classification of electrodes, concentration cells, liquid junction potentials – thermodynamic quantities from EMF data. Electrochemical energy – storage systems – primary and secondary batteries – fuel cells.

UNIT – IV

Electro Kinetic Phenomena

Electrical double layer potential –theory of multilayers at electrode – electrolyte interface – double layers capacity – electro kinetic phenomena – Zeta potential electro osmosis and sedimentation potential.

Process at electrodes – The rate of charge transfer – current density – Butler – Volmer equation – Tafel equation.

Principles of electrode position of metals – electrochemical corrosion metal constructions and use of Pourbaix and Evans diagrams and prevention of corrosion – Electrochemical oxidations and reduction.

UNIT – V

Surface Phenomena

Surface Phenomena: Terminology – Differences between adsorption and absorption- classification- Physisorption and chemisorption– solid – liquid interfaces, solid – gas interfaces,– Factors influencing adsorption of gases on solids- Adsorption isotherms- Freundlich's, Langmuir and BET isotherms – surface area determination. Applications of adsorptions-Activated carbon-application in the treatment of polluted water and other applications of activated carbon. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and membranes.

Reference:

1. S. Glasstone, Introduction to Electrochemistry
2. Vogel, A Textbook of Quantitative Inorganic analysis, Longman.
3. Bockris and Reddy, Electro chemistry
4. P.W. Atkins, Physical Chemistry, ELBS 6th edition.
5. A.K.Chandra, Introduction to Quantum chemistry
6. Donald.A.mcquarrie, Quantum chemistry
7. R.K.prasad, Quantum chemistry
8. Jain & Jain, Engineering Chemistry.

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credits
II	17P2CHC6	Physical Methods in Chemistry – I	5	5

UNIT I

Theoretical principles of Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecular systems. Transition moment integral and Oscillator strength. Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and nonrigid rotors, - Intensity of spectral lines, - Effects of isotopic substitution – Microwave spectra of polyatomic molecules – Linear and symmetric top molecules, Infrared spectra – diatomic and triatomic molecules, simple harmonic and anharmonic oscillators, - diatomic vibrating rotator, rotation-vibration spectrum of carbon monoxide, - Interaction of rotation and vibration (breakdown of Born – Oppenheimer approximation) – Influence of the rotation on the spectrum of polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations, Influence of nuclear spin.

UNIT II

NMR: ¹H NMR Spectroscopy – Multiplicity – Spin - spin splitting- Coupling constant – Vicinal and geminal coupling constants – Dependence of J on dihedral angle – Karplus equation – long range coupling constants, Influence of stereochemical factors on chemical shift of protons. First order and second order proton, Simplification of complex spectra – Double resonance techniques, shifts reagents. Chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH₂), an elementary treatment of NOE phenomenon. ¹³C NMR Spectroscopy – Basic theory of FT – NMR, – Broad band decoupling. Off resonance decoupling and chemical shifts of common functional groups.

UNIT III

UV –Visible and IR spectroscopy:

UV-Visible Spectroscopy:

Introduction - Instrumentation, Sampling techniques - Woodward–Fieser and Scott rules for conjugated dienes and polymers, ketones, aldehydes, α,β-unsaturated acids, esters, nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

Infrared Spectroscopy: Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies – Both internal and external – quantitative studies. Hydrogen bonding – (intermolecular and intramolecular).

UNIT IV

Electron spin resonance spectroscopy: Basic principles – comparison between esr and nmr spectra – hyperfine splitting – factors affecting the magnitude of g values – calculation of unpaired electron density on an atom in a delocalized system – applications to organic free radicals.

Mass Spectrometry: Instrumentation – Resolution, EI and CI methods – Base peak, isotopic peaks, metastable peak, parent peak, recognition of molecular ion peak – FAB. Fragmentation – General rules – Pattern of fragmentation for various classes of compounds, McLafferty rearrangements.

UNIT V

X-ray diffraction: X-ray diffraction by single crystal – Space groups –Systematic absences in X-ray data and identification of lattice types , glide planes and screw axes.X-ray intensities, structure factor and its relation to intensity and electron density , phase problem.

Electron Diffraction by gases - Scattering intensity vs Scattering angle, wierl equation, measurement technique.

Neutron diffraction by crystals – magnetic scattering, measurement techniques.

Application of IR, UV, NMR and Mass spectroscopy in the structural elucidation of organic compounds (Minimum 15 problems should be worked out).

References:

1. C.N. Banwell, Fundamentals of molecular Spectroscopy, 3rd ed., TMH, New Delhi, 1983.
2. B.P. Straughan and S.Walker Spectroscopy Vol.3, Chapman Hall London, 1976.
3. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.
4. P.K.Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
6. P.M. Silverstein, F. X. Wester, Spectroscopic Identification of Organic Compounds, 6th ed., Wiley 1998.
7. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
8. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1965.
9. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications, S.Chand,1992.
10. P.S.Kalsi, Spectroscopy of Organic Compounds.
11. Clegg,W., Crystal structure determination, Oxford University press , New York,1998.
12. Stout,G.H., Jensen , L.H. X-ray structure determination : A practical guide , John wiley & sons Publication: New York,1989
13. Glusker, J.P., Trueblood,K.N. Crystal structure analysis: A primer., Oxford university press, New York, 1972.

Web Pages:

Cambridge Structural Database (CSD)-<http://www.ccdc.cam.ac.uk/products/csd/>

Protein Data Bank (PDB) <http://www.rcsb.org/pdb/home/home.do>

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credit
II	17P2CHC7	Polymer chemistry	5	4

UNIT – I

Physical Properties and applications of Polymers: Mechanical – Stress – strain measurements, Electrical – conducting polymer – polyacetylene, polyaniline. Industrially important polymers – Natural and synthetic rubber – polyesters, polytetrafluoroethylene, (TEFLON), Polystyrene, ion-exchange Resins, polyacrylonitrile – carbon fibres, polyvinyl chloride and polyacrylates.

UNIT – II

Synthesis and Kinetics: Kinetics of polymerization – free radical chain polymerization, cationic polymerization, anionic polymerization, copolymerization, Degree of polymerization, chain length, chain transfer, chain termination, stereo regular polymerization, zeigler Natta catalysts.

UNIT – III

Characteriation: Crystalline Nature – X-ray diffraction, study of polymers, degree of crystallinity, Differential scanning Calorimetry, Thermogravimetric analysis of polymers. Glass Transition Temperature – factors affecting Glass Transition Temperature, properties associated with Glass Transition Temperature, Crystallinity and Melting point – Relations to structure.

UNIT – IV

Chemical Reaction Cyclization: Hydrolysis, Acidolysis, Hydrogenation, Addition and substitution reaction cross linking – Vulcanization, graft and Block Copolymers. Type of degradation – Thermal, Mechanical, Oxidative, Hydrolytic and photo degradation.

UNIT – V

Classification and Molecular weight Determination: Basic concepts of polymer science – molecular forces and chemical bonding in polymers – classification of polymer – addition polymers, condensation. Major mass and size of polymers – Number average and weight average molecular weight – methods of molecular weight determination. Osmometry viscosity, light scattering, sedimentation, Ultra centrifuge; Molecular weight distribution curve

References:

1. V.R. Gowariker – polymer science, wiley Eastern, 1986
2. K.J. Saunders, Organic Polymer Chemistry – Chapman and Hall, 1976
3. Raymound, B. Seymour, Polymer Chemistry – An introduction, Marcel Dekker Inc. NY 1981.
4. Fred W. Billmeyer – Text book of polymer science, john – wiley.
5. K. Gupta, fundamentals of polymer science and Engineering, Tata, McGraw Hill.
6. Stepak, polymer characterization of processing technology, Academic press, Indian.

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credits
II	17P2CHCP2	Physical Chemistry Practical-II (Electrical)	5	3

ELECTRICAL

1.CONDUCTOMETRIC TITRATIONS

I.acid – base titrations

- i) Strong acid Vs strong base
- ii) Weak acid Vs strong base
- iii) Mixture of acids Vs strong base
- iv) Mixture of bases Vs strong acid

II. precipitaion titrations

- i) KI Vs AgNO₃
- ii) Mixture of halides (KCl + KI) Vs AgNO₃
- iii) K₂ SO₄ Vs BaCl₂

III. verification of ostwald's dilution law

IV. Verification of Debye Huckel Onsagar equation

V.determination of solubility of sparingly soluble salt.

2. POTENTIOMETER TITRATIONS

I. acid – base titrations

- i) Strong acid Vs strong base
- ii) Weak acid Vs strong base
- iii) Mixture of acids Vs strong base

II. precipitation titrations

- i) KI Vs AgNO₃
- ii) Mixture of halides (KCl + KI) Vs AgNO₃

III .Redox titrations

- i) KMnO₄ Vs KI, FAS
 - ii) K₂Cr₂O₇ Vs KI, FAS
- IV. Determination of pH of buffer solutions
- V. Determination of activity coefficient
- VI. Determination of dissociation constant of an organic acid
- VII. Determination of Redox potential of Fe³⁺ / Fe²⁺ system

Semester	Subject code	Title of the paper	Hours of Teaching /Week	No. of Credits
II	17P2CHEL2A	Major Elective-II Paint Chemistry	5	4

UNIT – I

Paint ingredients : – Classification of paints – according to drying mechanism – under coats – Technical terms , Sag, Skin Irreversible gel, shelf life, Pot life, Solids, vehicle – consistency of thixotropy – Dry film properties – Adhesion – gloss – flexibility – repair and renovation – Pigments – function (opacity, protective and Reinforcing) – classification – properties – optical – particle size and shape – refractive index – Tinting strength – Chemical reactivity – Bleeding characteristic Hiding power – Examples of pigments – zinc oxide – chrome greens – Lithophone selection of pigments – dispersion – colour matching.

UNIT – II

Classification of solvents – facts and theory – solvent – properties – boiling point and evaporation rate – uses of solvents –toxicity. Paint additives wetting and dispersing agents. Anti setting – anti – sag and bodying agents – Aluminum soaps – hydrogenated castor oil, modified clays – anti skinning agents – examples – anti flood and anti- float additives – factors influencing flooding and floating – Mildew – inhibitors – dispersing agents (anionic) stabilizing agents (Non ionic) Anti foam agents – thickening agents – preservatives – freezer stabilizers.

UNIT – III

Lacquers : Cellulose polymers – acrylic polymers – PMM merits and demerits – film former – industrial application – Emulsions – problems associated – making of Emulsion – merits and demerits – House – hold Emulsion suitable film former – solid content (or) Non Volatile Material (NVM) and Minimum Film Forming Temperature (MFFT) – Drying and semi drying oils – drying mechanism of conjugated and non conjugated Oil Paints – Phenolic resin – Alkyd resin –preparation – properties – House hold air drying alkyd resin – formulation of wood primer.

UNIT – IV

Polyester Rein: amino resin – uses of amino resin – self polymerization – co reaction –alkyd and polyesters –thermosetting alkyd – urea formuldehyae resin and melamine formaldehyde resin . Ployurethane – raw materials – isocyanate (TDI, MDI, HDI) Hazards of isocyanate – classification of polyurethanes urethane oil and urethane alkyd - Moisture cure urethane – blocked isocyanate system – two component - polyol type polyurethanes.

UNIT – V

Epoxy Resin - Manufacture and characterization – curing agents –two pack system – solventless finishes – flooring compounds – fiber glass laminates – single pack thermoplastic epoxy system – water dispersible coatings – powder coatings –Paint film defects -popping – blushing - cissing – yellowing – and orange peel effect.

References :

1. G.P.A. Turner –Principles of Paint Chemistry and Introduction to paint Technology Oxford & IBH Publishing & Co
2. Paint Film Defects by HESS's
3. Modern technology of surface coating & Varnishes by SSP
4. Paint, Lacquers, Enamels, Powder coating & Varnishes by SSP consultan

Semester	Subject code	Title of the paper	Hours of Teaching/Week	No. of Credits
II	17P2CHEL2B	Major Elective-II Cheminformatics	5	4

Unit I

Introduction to Cheminformatics: Introduction to cheminformatics, History and Evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular Modeling and Structure Elucidation.

Unit II

Representation of Molecules and Chemical Reactions: Nomenclature; Different types of Notations; SMILES coding; Matrix Representations; Structure of Molfiles and Sdfiles; Libraries and toolkits; Different electronic effects; Reaction classification.

Unit III

Searching Chemical Structure: Full structure search; sub structure search; basic ideas; similarity search; Three dimensional search methods; Basics of Computation of Physical and Chemical Data and structure descriptors; Data visualization.

Unit IV

Computer Assisted Virtual screening design: Structure Based Virtual Screening-Protein Ligand Docking, Scoring Functions for Protein Ligand docking, Practical aspects of structure based Virtual Screening; Prediction of ADMET Properties, 2 D and 3D data searching, Chemical databases, Role of computers in Chemical Research.

Unit V

Application of Cheminformatics in Drug Design: Quantitative Structure-Property Relations; Descriptor Analysis; Computer Assisted Structure elucidations; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Design of Combinatorial Libraries; LigandBased and Structure Based Drug design

Text Book

1 Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Cheminformatics, Academic Publisher, Netherlands, 2003.

Reference Books

1. Lisa B. English (Editor), Combinatorial Library Methods and Protocols, Humana Press Inc, Volume:201, 2002.
2. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition, 2006.

Semester	Subject Code	Title of the Paper	Hours of Teaching /Week	No. of Credits
III	17P3CHC8	Organic Chemistry – II	5	5

Unit -I: Electrophilic substitution

Aliphatic electrophilic substitution: SE₁, SE₂ and SE_i mechanism effect of substrate structure, leaving group, attacking electrophile and solvent. Stork-enamine reaction decarboxylation of aliphatic acids-halogenation of aldehydes and ketones.

Aromatic electrophilic substitution: Arenium ion mechanism-evidence-orientation and reactivity-nitration, halogenations, sulphonation, Friedel Crafts reactions-Formylation reaction-Gattermann, Gattermann-Koch, Reimer-Tiemann and Vilsmeier-Hack reactions.

UNIT II:

Reactive intermediates and methods of determining reaction mechanism

Generation, reactivity, structure and stability of Carbocations, Carbanions, Carbenes Nitrenes and arynes. **Free radicals** – Configurations – Identification by chemical and spectral methods – Free radical halogenation - NBS.

Mechanism and methods of determination: Thermodynamic and kinetic control-Hammond postulate-Microscopic reversibility-intermediate versus transition state.

Kinetics and non-kinetic methods of determining mechanism - Product analysis, Determination of the presence of intermediates-isolation, detection and trapping-crossover experiments-isotopic labeling, isotopic effects- stereo chemical evidence-kinetic evidence.

UNIT III: Addition and Elimination Reactions

Addition reactions: Addition to carbon-carbon multiple bond-mechanistic and stereochemical aspects of electrophilic, nucleophilic additions-orientation and reactivity-addition reaction of bromine and hydrogen bromide, hydroxylation, hydroboration, epoxidation oxymercuration, Michael addition. **Addition to carbonyl groups:** Mannich, Stobbe, Oppenauer oxidation, MPV reduction, Darzen's glycidic ester condensation, Wittig reaction.

Elimination reactions: E₁, E₂, E₁CB and E_i mechanism - stereochemistry of elimination, Hofmann and Saytzeff rules- competition between elimination and substitution - chugaev reaction-dehydration of alcohols - dehydro halogenations - Hoffman degradation-cope elimination - Bredt's rule with examples.

Unit IV: Molecular Rearrangement and Reagents

Molecular rearrangement: Mechanism of the followings - Wagner Meerwein, dienone-phenol, Wolf, Lossen, Schmidt, Bayer-Villiger, Stevens and Favorski rearrangements.

Reagents in organic synthesis: Complex metal hydrides, LiAlH₄, NaBH₄, tertiarybutoxy aluminium hydride, NaCNBH₃ and tri n-butyl tin hydride DIBAL-H. Lithium dimethyl cuprate, lithium di-isopropylamide, DCC, 1,3-dithiane, trimethyl silyl iodide, DDQ, SeO₂, Phase transfer catalysis, crown ethers.

Unit V: Pericyclic Reactions

Concerted reactions-stereochemistry-conservation of orbital symmetry-FMO method-selection rules-electrocyclic, cycloaddition and sigmatropic reactions-1,3 and 1,5 hydrogen shift-cope and claisen rearrangement - fluxional molecule. Woodward Hoffmann rule-correlation diagram method- electrocyclic and cycloaddition only.

References

1. J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and structure*, 5th ed. Wiley, 2000
2. Clayden, Greeves, Warren and Wothers, *Organic chemistry*, 2nd ed. Oxford University press.
3. Francis A. Carey and Richard J. Sundberg, *Advanced organic chemistry part A: Structure and Mechanisms*. 5th ed. springer
4. Francis A. Carey and Richard J. Sundberg, *Advanced organic chemistry part B*. 5th ed. springer
5. Peter Sykes, *A Guide book to Mechanism in organic chemistry*, 6th edition Longman, 1986
6. P.S.Kalsi, *Stereochemistry Conformation and mechanism*, 5th edition New Age international
7. V.K.Ahluwalia and R.K.Parashar, *Organic reaction mechanisms*. 3rd edition, Alpha Science Int'l Ltd
8. S.M.Mukherji and S.P.Singh, *Reaction mechanism in organic chemistry*. 3rd edition Macmillan India Limited.
9. Bhupinder Mehta and Manju Mehta "Organic Chemistry", PHI Learning Pvt Ltd, New Delhi – 110001.(2012)

Semester	Subject Code	Title of the Paper	Hours of Teaching/Week	No. of Credits
III	17P3CHC9	Physical Methods in Chemistry – II	5	5

UNIT I

Electronic Spectroscopy

Term symbols of atoms, ions and molecules – Microstates - energy levels for d1 – d9 ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra – Sugano Tanabe diagrams. Orgel diagram for d1 – d9 systems. Evaluation of $10Dq$ and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra.

Optical rotatory dispersion and circular dichroism Cotton effect and ORD curves. Axial haloketone rule, octant rule and its applications. Application of ORD to determine absolute configuration of simple monocyclic ketones.

UNIT – II

Infrared and Raman Spectroscopy

Vibrations in simple molecules (H_2O , CO_2) and their symmetry notation for molecular vibrations – Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O , ClF_3 , NO_3 , ClO_4 – effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) – Applications of Raman Spectroscopy – Resonance Raman Spectroscopy.

UNIT – III

NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (1H , ^{19}F , ^{31}P , ^{13}C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (2H , ^{10}B , ^{11}B) on the 1H NMR spectra.

Systems with chemical exchange - study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions.

UNIT IV

EPR spectroscopy

Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of V(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

Magnetic properties:

Types of magnetism – Dia – para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states KT – states $\ll KT$. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides.-orbital contribution to magnetic moment, range of μ_{eff} for various complexes gouys method Spin crossover in coordination compounds.

UNIT V

Mossbauer Spectroscopy

Isomer shifts – Magnetic interactions – applications to iron and tin compounds.

NQR spectroscopy

Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

REFERENCES:

1. R.S.Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company.
2. R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Company, Philadelphia, London.
3. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company New Delhi 1990.
4. P.J. Wheatley, The Determination of Molecular Structure, .
5. Lewis and Wilkins, Modern Coordination Chemistry, .
6. E.A.V.Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.

M.Sc. Chemistry

Semester	Subject Code	Title of the Paper	Hours of Teaching/ Week	No. of Credits
III	17P3CHC10	Industrial Chemistry	5	5

Unit I

Basic ideas about unit operation – Flow Chart – Chemical Conversion – Batch versus Continuous process – Chemical Process selection – Design – Chemical Process Control – Chemical process of economics- market evaluation – Plant location- Management for productivity activity – Research & Development and its role in chemical industries.

Unit – II

General Survey of chemicals used in everyday life, Cosmetics – talcum powder, tooth paste, shampoo – nail polish – Perfumes – Soaps and detergents – General Formulation and preparation – Hazards of cosmetic use.

Unit – III

Food and Nutrition – Carbohydrates – Proteins fats, minerals and Vitamins – Definition sources and their physiological importance – balanced diet – Adulterants in Milk – Ghee – Oil – Coffee powder – Chili Powder – Pulses – Turmeric powder – identifications.

Unit – IV

Plastics – Polythene – PVC, Bakelite, Polyester resin – properties and applications, Natural rubber, Synthetic rubber – Vulcanization – Classification and its applications – Color chemicals used in food – soft drinks and its health hazard.

Unit – V

Manufacture of Cement, Introduction – Types of cement – high alumina cement – Water proof cement – slag cement- acid resisting cement – White cement – colored cement – pozzolana cement – setting of cement – properties of cement – testing of cement – uses of cement – concrete -cement Industries in India.

References:

1. Norrish Shreve. R. and Joseph A. Brink Jr Chemical Process Industries, McGraw Hill, Industrial Book Company London.
2. Mohapatra – elements of Industrial chemistry 1988 in Delhi – Kalyani publications.
3. B.K.Sharma Industrial Chemistry 1st edition – Goel publications – Meerat 1983.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
III	17P3CHCP3	Organic practical-I	5	3

1. Qualitative analysis of organic mixture:

- a. Pilot separation
- b. Bulk separation
- c. Analysis
- d. Derivative

2. Separation of amino acids using paper chromatography

3. Separation of organic compounds using TLC (CIA) only

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
III	17P3CHCP4	Organic practical-II	5	3

I. Estimations

Estimation of phenol

1. Estimation of aniline
2. Estimation of ketone
3. Estimation of glucose
4. Estimation of Ascorbic acid

II. Two Stage Preparations:

1. Preparation of m-nitro benzoic acid from methyl benzoate
2. Preparation of p – nitro aniline from acetanilide
3. Preparation of aspirin from methyl salicylate
4. Preparation of p-bromoacetanilide from aniline

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
IV	17P4CHC11	Inorganic Chemistry - II	6	6

UNIT – I

Co-ordination Chemistry: Nomenclature of mono and polynuclear complexes – Crystal field theory – shapes of d orbitals in octahedral symmetry – Splitting in tetrahedral symmetry – only weak field splitting – reasons. Tetragonal symmetry – differences between tetrahedral and tetragonal symmetry. CFSE – Strong Field and weak field splitting – Calculation of CFSE for d^1 to d^{10} system. Splitting pattern in trigonal, square planar, trigonal bipyramidal, square pyramidal & cubic symmetries. Factors affecting the magnitude of splitting ($10 Dq$) – spectro chemical series. Jorgensen's principles. Evidences for CFT. Jahn – Teller distortion – Magnetism and colour of transition metal ions, LFT, Nephelauxetic effect.

M.O. Theory – Octahedral, tetrahedral and square planar complexes. Pi bonding and M.O. theory – ligands having filled and empty pi bonds – effect on $10 Dq$. Evidences for pi bonding from X-ray Crystallography, IR spectroscopy.

UNIT – II

Stability of Co-ordination compounds:

Labile and inert complexes - Detection of complex formation in solution, stability constants, stepwise and overall formation constants – pH metric, polarographic and photometric methods of determining of formation constants. Factors affecting stability – statistical and chelate effects.

Kinetics and mechanisms of reactions in solutions:

Ligand displacement reactions – hydrolysis, equilibrium in octahedral and square planar complexes – Trans effect. Electron transfer reactions – Complementary and non-complementary types – inner sphere and outer sphere processes – isomerisation and racemization. Reactions of coordinated ligands, Template effect and syntheses of macro cyclic ligands.

UNIT – III

Inorganic Photochemistry – Electronic transitions in metal complexes – Various photophysical processes of coordination compounds – Photosubstitution, photo isomerisation, photo oxidation, photo reduction photochemistry of chromium (III) complexes. Adamson's rule – photochemistry of organometallic compounds, metal carbonyl compounds.

Main group element -Periodicity--first and second row anomalies-size effect in non metals-diagonal relationship - nitrogen phosphorous analogies and contrasts- $P\pi$ – $P\pi$ bonding in heavier non metals.The use of d orbitals by nonmetals-theoretical arguments against d orbital participation in nonmetals-experimental evidence for bonding.

UNIT – IV

Complexes of pi-acceptor ligands – Carbonyls – 18 electron rule – Isolobal concept – application to structure of carbonyls (simple and polynuclear). Carbonylate anions, carbonyl hydrides. Nitrosyl complexes – bridging and terminal nitrosyls – Bent and linear dinitrogen complexes -Metallocenes – reactions – Catalysis by organometallic compounds-ferrocene-hapticity-carbene complexes-fluxional molecule. Hydrogenation

and Hydroformylation of olefins – Oxidation of olefins to aldehydes and ketones – polymerization of alkenes cyclo – oligomerisation of acetylene – Fischer – Tropsch synthesis.

UNIT – V

Bio-inorganic Chemistry

The biological roles of metal ions, calcium biochemistry, oxygen transport and storage, chlorophyll - carbonic anhydrase, carboxypeptidases, Fe-S proteins and non-heme iron cytochromes of the electron transport chain, cytochrome P-450 enzymes, coenzyme B12, nitrogen fixation and photosynthesis. Metal chelation and the activity of the multipurpose drug.

Anticancer Activity of Platinum Complexes: Different types of active Pt-complexes; toxic effects of anticancer Pt-complexes; mechanism of anticancer activity; nonactivity of trans-platin.

Reference:

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic Chemistry* 4th ed., Addison – Wesley (Unit I, II, III, IV)
2. A.W. Adamson, *Inorganic photochemistry* (Unit – III)
3. Keith F. Purcell and John C. Kotz, *Inorganic Chemistry*, Saunders Golden Sunburst Series, W.B. Saunders Company, Philadelphia, 1977.
4. W. Kain and B. Sehwerski, *Bio – Inorganic Chemistry; Inorganic Elements in the Chemistry of life*, John Wiley & Sons, New York.
5. Shriver, Alkins and Longford, *Inorganic Chemistry*, ELBS, 1994 (Unit II).
6. Asim K. Das, *Bioinorganic Chemistry*, 2008.

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
IV	17P4CHCP5	Inorganic Practical – I	6	3

Qualitative Analysis of common and less common cations by Semi – micro technique in mixtures

Common Cations :

Lead Bismuth, Copper, Cadmium, Antimony, Tin, Iron, Aluminum, Chromium, Manganese, Nickel, Cobalt, Zinc, Calcium, Barium, Strontium, Magnesium and Ammonium.

Less Common Cations :

Tungsten, Thallium, Selenium, Tellurium, Molybdenum, Cerium, Thorium, Zirconium, Beryllium, Uranium, Lithium.

I. Colorimetric Estimation of Copper, Iron, Chromium and Nickel

Semester	Subject code	Title of the paper	Hours of Teaching/ week	No. of Credit
IV	17P4CHCP6	Inorganic Practical – II	6	3

I. ESTIMATIONS OF MIXTURE SOLUTIONS

1. Estimation of Copper and Zinc
2. Estimation of Iron and Nickel
3. Estimation of Copper and Nickel
4. Estimation of Calcium and Magnesium

II. Preparation of the following Inorganic Complexes

1. Lead tetra acetate
2. Bis (pyridinium hexa chloroplumbate
3. Tris (thiourea) copper (II) sulphate
4. Potassium bis (oxalate) aluminate (II)
5. Hexathiourea lead (II) nitrate
6. Potassium bisoxalato diaquo chromate (III)
7. Hemannine cobalt (III) chloride.

Semester	Subject code	Title of the paper	Hours of Teaching/Week	No. of Credits
IV	17P4CHEL3A	Major Elective - III Recent Trends in Chemistry	6	4

Unit – I

Nano Chemistry – Introduction – discovery of CNT, preparation of CNT – arc method – laser ablation method – chemical vapour deposition method, properties – thermal, mechanical, optical, electrical and other properties – uses of CNT. Nano sensors – chemical sensors and biosensors and their uses. Uses of nanotechnology in computers solar energy, fuel cells, medicine and metallurgy.

Unit - II

Nano Synthesis - Preparation of nano materials by micro wave synthesis – sol-gel method – chemical co-precipitation – hydrothermal and solvothermal methods. Preparation and uses of TiO₂ and ZnO. Fullerene – preparation – properties and uses. Principle and uses of AFM. Implications of nano science and nano technology on society. Nano shells and their applications.

Unit – III

Green Chemistry – Introduction, Designing of green synthesis – choice of starting materials, reagents, catalysts and solvents. Twelve principles of green chemistry and their explanation with examples.

Biocatalysts in organic synthesis: Introduction–oxidoreductases-transferases –hydrolases-lyases-isomerases-ligases. biochemical oxidations and biochemical reductions-applications

Unit – IV

Green reagents – dimethyl carbonate, polymer supported reagents – (eleven reagents). Green catalysts – acid catalysts, oxidation catalysts, basic catalysts, and polymer supported catalysts – polystyrene aluminium chloride, polymeric super acid catalysts, polymer supported photo sensitizers and phase transfer catalysts. Ionic liquids as green solvents – reactions in acidic ionic liquids and neutral ionic liquids, hydrogenation, Diels – Alder reaction, Heck reaction, O-alkylation and N-alkylation, Methylene insertion reactions.

Unit – V

Supra Molecular Chemistry – Concepts and Languages of supramolecular Chemistry – Supramolecular Reactivity and Catalysis.

Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophanes. Type Receptors. Supramolecular Metallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis.

Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimers, Gelators. Classification and typical reactions- Applications.

References:

1. New Trends in Green Chemistry by V.K. Ahluwalia & M. Kidwai, Anamaya publishes, New Delhi.
2. Chemistry for Green Environment by M.M. Srivastava, Rashmi Sanghi, Narosa publishers, New Delhi.
3. Nano the Essential by T.Pradeep. Tata Mc Graw Hill Education Private Limited, New Delhi.
4. Supramolecular and cluster chemistry by John.
5. Environmental chemistry by B.K.Sharma
6. Bioorganic, bioinorganic and Supramolecular chemistry by P.S.Kalsi and J.P kalsi.
7. Supramolecular chemistry–Fundamental and application by katsuhikoariga – Toyaki Kunitake

Semester	Subject Code	Title of the Paper	Hours of Teaching / Week	No. of Credits
IV	17P4CHEL3B	Major Elective – III Applied Chemistry	6	4

Unit-I: Dye Chemistry

Pretreatment: Sizing, Desizing- acid method, Scouring- kier boiling method, Bleaching – hypochlorite method, Mersirization, fastness properties – washing, rubbing and light fastness

Dyeing: Dye fibre bond, % of shade, M:L ratio, % Of exhaustion, equilibrium absorption, effect of electrolyte.

Reactive dye - principles of dyeing. **Polyester dyes** - carrier dyeing - mechanism and high temperature dyeing. **Mordant dyes** – principles – specific examples **Acid dyes**-dyeing mechanism – role of electrolyte and dye bath assistants **Vat dyes** – vatting – dyeing – oxidation and after treatment

Unit-II: Paint Chemistry

Paint – definitions – ingredients and their role – terminology – emulsion, lacquer. Enamel – pot life, shelf life –varnish – thixotropy –classification of paints based on drying mechanism - under coats – Pigments – classification (organic & inorganic) – functions – properties such as hiding power, light fastness, particle size and shape Solvents used for paints – flash point.

Vehicles: Oil – drying mechanism, Description of Alkyd, Epoxy, Polymethyl methacrylate, Urea formaldehyde, Melamine formaldehyde, urethane resins. Additives – Anti skinning agents Powder coating, Solvent less finish.

Unit- III Sonochemistry

The use of Ultrasound in Organic synthesis

Introduction – Instrumentation – The physical aspects – Types of Sonochemical reactions – Homogeneous reactions – Heterogeneous liquid – liquid reactions – Heterogeneous solid – liquid reactions – Synthetic Application – Esterification – Saponification – Hydrolysis / Solvolysis – Substitutions – Addition reactions – Alkylations – Oxidation – Reduction – Hydroboration – Hydrosilation and hydroalkylation – Coupling reactions – Dichlorocarbene – Other Reactions – Bourgveault reaction – Cannizzaro reaction – Strecker synthesis – The Reformatsky reaction – The barbier reaction of carbonyl compounds – Condensations – Carbohydrates – formation of acetals and benzylidene derivatives of alkylglycopyranosides.

Unit – IV

Bio Organic Chemistry – Introduction – definition – Branches of Bio chemistry – Scope – Biomerkenes – functions.

Carbohydrate – Introduction – Classification, Mutarotation, Pyronose form, furanose form, Glycogen – structure. **Protein** – Introduction – Classification structure.

Vitamins – Introduction – Source structure – deficient diseases of B₁, B₆, B₁₂, A, D– Uses classification. **Alkaloids** – Introduction– occurrence classification. **Nucleic Acid** – RNA, DNA – types of RNA – Differences – Structure of DNA.

Unit – V

Medicinal Chemistry - Mechanism of drug action and Metabolism of Drugs: Mechanism of action – Drug Receptors and Biological responses – Mechanism of different types of drug action – Metabolism of drugs – Chemical pathway of drug metabolism absorption of drugs – Routes of administration - factors affect absorption – Digestion and absorption of protein – Digestion of fat.