ST. XAVIER'S COLLEGE (AUTONOMOUS)

(Recognized as "College with Potential for Excellence" by UGC)
(Accredited by NAAC at "A^{++}" Grade with a CGPA of 3.66 out of 4 in IV Cycle)
(Star College Programme by DBT, Govt. of India.)

Palayamkottai - 627 002

SYLLABUS

Preserve this copy of the syllabus until you complete the course, as it is an important document of your present course of study.

Name _____

M.Sc. CHEMISTRY

Choice Based Credit System (CBCS)
(w.e.f. June 2021 - 22)

Programme Outcomes (PO):

The Post graduate students passing out from St. Xavier's College will be able to

- **PO 1:** To acquire expertise in their own discipline
- **PO 2:** To identify, formulate, perform research literature survey and analyze complex problems
- **PO 3:** To come out with substantial conclusions using principles of all branches of sciences, commerce, economics and Management.
- **PO 4:** To develop Specific skills in Planning and Conducting advanced experiments recording and analyzing the data and draw the relevant conclusions from it.
- **PO 5:** To collaborate in order to analyze and find solutions of existing problems of India and the World.
- **PO 6:** To establish themselves in hot areas of research and contribute to the developmental needs of India and the World.
- **PO 7:** To become Knowledge transfer agents of the Society
- **PO 8:** To become employable in Science, Education, Technology R&D, Finance and Commercial sectors.

COURSE PATTERN PG – Science Programmes: Hours and Credit allotments

Sem	Papers	Subject Code	Title	Hours	Credit
I	Core – I	21PGCH11	Organic chemistry – I	5	5
	Core – 2	21PGCH12	Inorganic chemistry – I	5	5
	Core – 3	21PGCH13	Physical chemistry – I	5	5
	Elective – 1	21PGCHE11	Selected topics in Inorganic chemistry and Supramolecular chemistry / Chemistry of Natural products	5	5
	Practical – 1	21PGCHP11	Physical chemistry Practical-I	4	2
	Practical – 2	21PGCHP12	Organic chemistry Practical – I	2	1
	Practical – 3	21PGCHP13	Organic Chemistry Practical –II	2	1
	Library Seminar			2	-
			Sub-Total	**30**	**24**
II	Core - 4	21PGCH21	Organic chemistry – II	5	5
	Core – 5	21PGCH22	Inorganic chemistry –II	5	5
	Core – 6	21PGCH23	Physical chemistry – II	5	5
	Elective – 2	21PGCHE21	Pharmaceutical chemistry / Current Trends and Research Techniques in Medicinal Chemistry	5	5
	Practical – 1	21PGCHP21	Physical chemistry Practical-II	4	2
	Practical – 2	21PGCHP22	Inorganic chemistry Practical – I	2	1
	Practical – 3	21PGCHP23	Inorganic Chemistry Practical – II	2	1
			Sub-Total	**30**	**24**
			Internship	**-**	**2**
III	Core – 7	21PGCH31	Organic chemistry – III	5	5
	Core – 8	21PGCH32	Inorganic chemistry –III	5	5
	Core – 9	21PGCH33	Physical chemistry – III	5	5
	Elective – 3	21PGCHE31	Research Methodology /Cheminformatics	5	5
	Practical – 5	21PGCHP31	Inorganic chemistry Practical – III	4	2
	Practical – 6	21PGCHP32	Inorganic chemistry Practical – IV	2	1
	Practical – 7	21PGCHP33	Organic Chemistry Practical –III	2	1
	Practical – 8	21PGCHP34	Organic Chemistry Practical –IV	2	1
	Library/seminar			2	-
			Sub-Total	**30**	**24**
IV	Core – 10	21PGCH41	Selected topics in chemistry	5	4
	Core – 11	21PGCH42	Emerging Trends in Physical chemistry	5	4
	Core-12	21PGCHS41	Comprehensive chemistry	-	2
	Elective -4	21PGCHE41	Analyticaland Green chemistry / BioChemistry	4	2
	Project	21PGCHD41	Dissertation	10	4

	Practical – 7	21PGCHP41	Physical chemistry Practical – III	4	2
	Library Seminar			2	-
	STAND			-	1
			Sub-Total	30	19
			Grand Total	**120**	**91**

EXTRA CREDIT COURSES

Semester	Course Code	Title of the Course	Hours	Credits
I	21PGCHECC11	Industrial Chemistry	-	2
II	21PGCHECC21	Environmental Chemistry	-	2
III	21PGCHECC31	Health Chemistry	-	2
IV	21PGCHECC41	Analytical Chemistry	-	2

Programme: M.Sc. Chemistry
Programme Code: PCH
Programme Specific Outcomes:

By the completion of the M.Sc. ChemistryProgramme, the student will be able to

- **PSO1:** realize the concepts in organic, inorganic, physical, pharmaceutical, computational and analytical chemistry and apply them in their higher studies research.
- **PSO2:** identify, reason out, formulate and solve the complications and modernize chemicalindustriesby applying the concepts of chemistry.
- **PSO3:** design, develop and demonstrate the research problems related to health, industrial,global, social and environmental issues.
- **PSO4:** defend the findings of research by communicating effectively and deliver messages and suggestions in national, international level seminars/symposium and conferences with the aid of ICT tools.
- **PSO5:** play the role of team leader and imbibe the value-based behaviors such as tolerance, to carry out research in team.
- **PSO6:** be a responsible citizen with ethical and human values in research and related fields.
- **PSO7:**progress as enduring learners in their chosen carriers and update the recent developments in both chemistry and allied fields in science and technology.

CORE – ORGANIC CHEMISTRY – I (THEORY)

(Subject code: 21PGCH11)

Semester: I	Core: 1	Hours/W: 5	Credits: 5

Course Outcome:

By the end of the Course the student will be able to

CO 1: acquire an elaborate knowledge in the various effects operating in organic reactions and in chemical bondings (K1)

CO 2: classify the aromatic and non-aromaticcompoundsapplying Huckel's & Craig's rule(K4)

CO 3: apply stereochemical rules to predict the configuration and optical activity(K3)

CO 4: explain the mechanism of Aliphatic and Aromatic Nucleophilic substitution reactions (K2)

CO 5: evaluate the use of reagents in organic synthesis (K5)

CO 6: design the innovative reagents and propose mechanism for the organic synthesis(K6)

Unit I Basic concepts in Organic Chemistry **15 hrs**

Basic Concepts of electronic effects- Inductive effect- Field effect, Resonance, Electronic substituent effect on intermediates, Aromaticity, Concept of aromaticity, Homoaromaticity, Antiaromaticity, Huckel's rule- Aromaticity of azulene, tropolone, annulene and sydnone.

Self Study: acidity of cyclopentadienide anion

Unit II Stereochemistry **15 hrs**

Stereochemistry - Concept of chirality,Chirality - Prochiral centre, Prochiral face, Homotopic,Enantiotopic and diastereotopic ligands,Enantioselective hydrogenation,Double Stereo differentiation -Reinforcing and competing stereo selectivity - Asymmetric synthesis - Cram's rule and Prelog's rule (Craig and Baldwin rule) - E/Z notation of compounds containing one and two double bonds - Conformational analysis of cyclohexane - Effects of hydrogen bonding, dipole and steric effects on the conformation of disubstituted cyclohexanes - Atropisomerism in biphenyls, spiranes and allenes - R/S nomenclature for biphenyls, spiranes and allenes - Conformation of cis and trans decalin

Self Study:Re/Si nomenclature.

Unit III Aliphatic Nucleophilic Substitution Reaction **15 hrs**

General methods of investigating reaction mechanism - Principle of microscopic reversibility - Kinetic and thermodynamic controlled reactions - Hammond postulations, HAMMETT equation- significance of σ, σ* rho-Taft equation- applications of Hammett and Taft equation - Kinetic isotopic study - Isotopic labeling – cross-over experiment - Nucleophilic substitution at the saturated carbon atom: S_N1 , S_N2, S_Ni , S_N2 , S_N1 and S_Ni mechanisms - Curtin Hammett Principle- Effect of substrate, nucleophile, leaving group and the solvent on the rate of substitution reactions - neighboring group participation (phenyl, double bond and acetoxy group only). Mechanism of esterification and ester hydrolysis

Self Study: SET Mechanism

Unit IV Aromatic Nucleophilic Substitution Reaction and Addition to Carbon – Carbon Multiple Bonds 15 hrs

Aromatic nucleophilic substitution reaction - Unimolecular – bimolecular benzyne mechanisms - Addition of hydrogen - Catalytic hydrogenation – Birch reduction - Dieckmann condensation - Mannich reaction -Robinson annulation reaction - Wittig reaction - Sharpless asymmetric epoxidation - Addition of halogen and hydrogen halides to carbon-carbon double bonds - Acid catalyzed hydration and related addition reactions - Michael addition

Self Study: Simon-Smith reaction

Unit V Reagents in organic synthesis 15 hrs

Reagents in Organic Synthesis:SeO_2, $KMnO_4$, OsO_4, HIO_4,DDQ,NBS and m-CPBA,Reduction involving complex metal hydrides DIBAH, Tri – n-butyl tinhydride, Baker yeast. Phase transfer catalysts, crown ether,LDA, $(CH_3)_3SiI$,Aluminiumisopropoxide, diazomethane, Organo rhodiumcompounds.AIBN, Gilman reagent, Merrifield resin, Collin's reagent, 1,3-dithiane and CAN.

Self Study:Organo Lithium and Organo Copper compounds.

REFERENCES

UNIT I

1. Clayden, Greeves, Warren and Wothers-Organic Chemistry,Oxford University press
2. Jerry March – Advanced Organic Chemistry, 4th Edition, Reprint 2003, Wiley.

UNIT II

1. E.L.Eliel, "Stereochemistry of Carbon Compounds", 2003, A Wiley interscience publication.
2. I.L. Finar, "Organic Chemistry", Vol.II, 4th Edition, Indian Reprint 2005, Pearson Education.
3. D.Nasipuri, "Stereochemistry of Organic Compounds", Reprint 2002, New age International publishers.
4. K. Mislow – Introduction to Stereochemistry, 1966, Benjamin.

UNITS III& IV

1. Jerry March – Advanced Organic Chemistry, 4th Edition, Reprint 2003, Wiley.
2. P.S. Kalsi, "Organic Reactions Stereochemistry and Mechanism"New Age International Publishers.
3. Francis A. Carey and Richard J. Sundberg, "Advanced Organic Chemistry", 4th Edition, 2001, KluwerAcademic publishers.
4. V.K. Ahluwalia and R.K. Parashar, "Organic Reaction Mechanisms", 3rd Edition, Narosa publishing house.
5. R.M. Acheson – Chemistry of Heterocyclic compounds, 1973, Wiley Eastern.

6. I.L.Finar – Organic Chemistry, vol.II, 4th Edition, Indian Reprint 2005, Pearson Education.
7. S.M. Mukherji and S.P. Singh, "Reaction Mechanism in Organic Chemistry", Macmillan India. Ltd.
8. V.K. Ahluwalia and R.K. Parashar, "Organic Reaction Mechanisms", 3rd Edition, Narosa publishing house.

UNIT V

1. I.L. Finar, Organic Chemistry, Vol. I & II,3rdIndian Reprint, 2001, Pearson Education.
2. R.O.C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3rded., CRC Press, Taylor and Francis Company.

INORGANIC CHEMISTRY – I
(Subject code:21PGCH12)

Semester: I	Core:2	Hours/W:5	Credits:5

COURSE OUTCOME:

By the end of the Course the student will be able to

CO 1: summarize the fundamentals and describe the structure of solids (K2)

CO 2: predict the crystal defects and show the bonding in metals(K3)

CO 3: Predict the structures of molecules using VSEPR theory(K3)

CO 4: analyze the importance of Pearson's principle in acid-base concepts(K4)

CO 5: Justify the variations in periodic properties, crystal lattices, feasibility of chemical reactions in non-aqueous solvents(K5)

CO 6: integrate the ideas of ionic and covalent bonding in various molecules.

Unit I: Solid State Chemistry – I **15hrs**

Elements of crystallography - Space lattices and unit cell, Crystal system, X-ray diffraction - Bragg's method, Rotating crystal method, Powder method, Structure of typical lattices,AX type - Cesium chloride, Zinc Blende, Wurtzite, Nickel Arsenide. AX_2 type - Rutile, fluorite, antifluorite, CdI_2. ABX_3 type- Perovskite, AX_3 type- ReO_3. Covalent crystals – diamond and graphite

Self-Study: Close packing of solids

Unit II: Solid State Chemistry – II **15hrs**

Crystal defects- Line defect and point defects- Stoichiometric defects- Schotky and Frenkel defects- Non – stoichiometric defects- Electronic structure of solids- Free electron theory, Band theory- Types of solids – Conductors, Insulators, Semiconductors- Intrinsic semiconductors, Extrinsic semi-conductors, Photo excited semi-conductors. Super conductors – BCS theory- High and Low temperature superconductors.

Self-Study:Polymorphism of metals, Josephson Effect

Unit - III: Acids and Bases **15hrs**

Acid base concepts- Bronsted-Lowry, Lux-Flood, Usanovich, Lewis, solvent system and generalized acid base concepts. Measures of acid – base strength-Steric effect and solvation effects- Hard and soft acids and bases – acid base strength and hardness and softness. Symbiosis.

Solvents – classification of solvents.Typical reactions in non – aqueous solvents like liquid NH_3, liquid SO_2, liquid HF and H_2SO_4

Self-Study:Super acids and Super bases, Non aqueous solvent-N_2O_4

Unit-IV: Ionic Bonding **15hrs**

Ionic bond and its characteristic features-Lattice energy, Born-Lande equation, Born Haber cycle and its applications (NaCl, KCl,$MgBr_2$).Radius ratio rule - Polarization-Fajan'srule - results of polarization. Electronegativity – determination- Pauling, Mulliken, Jaffe scales- methods of estimating charges, electronegativity equalization, Types of chemical forces- Effects of chemical forces - melting and boiling points, solubility and hardness.

Self-Study: Kapustinskii equation and Allen electronegativity scale

Unit -V: Covalent Bonding **15hrs**

Valence bond theory - Resonance- Formal charge - Hybridization - Hybridisation and Overlap

MO theory-Symmetry and overlap-Molecular Orbitals in homonuclear diatomic molecules - B_2, C_2, N_2 and O_2-MO of heteronuclear diatomic molecule - CO and HCl,MO of triatomic molecule – BeH_2- MO of polyatomic molecule- NH_3

VSPER Theory and its applications- CO_2, $B(CH_3)_3$, $COCl_2$, POF_3, PF_5, SF_6, $[NH_4]^+[BF_4]^-$, Al_2Br_6, CH_4, NH_3,H_2O, SF_4, BrF_3, ICl_2-, TeF_5- , ICl_4-, IF_7, XeF_2, XeF_4, XeF_6, XeO_3, XeO_4, XeO_2F_2, $XeOF_4$. Bent's rule (PCl_3F_2) and the energetics of hybridization**.** Berry pseudo rotation

Self-Study:Hydrates and Clathrates

REFERENCES:

1. L.Azaroff , "Introduction to Solids", 3rd edition, 1977, Tata Mc-Graw Hill.
2. M.G.Arora, Solid state chemistry, 2001, Anmol Publication Pvt. Ltd., New Delhi.
3. Addison.W.E., Structural principles of Inorganic chemistry,1961, WilleyInterscience, New York.
4. Anthony R West., "Solid state chemistry and its applications", John Willey&sons (Asia)Pvt. Ltd.
5. Sisler, Chemistry in non – aqueous solvents, 1961, Reinhold publishing Corporation.
6. James E. Huheey, Inorganic Chemistry, Principles of structure and reactivity,4th edition, Pearson education.
7. J.D.Lee, Concise Inorganic Chemistry, 5th edition, 1996, Blackwell Science Ltd.
8. F.A.Cotton and G.Wilkinson – Advanced Inorganic Chemistry, 3rd edition, Pearson education.

CORE – PHYSICAL CHEMISTRY – I (THEORY)

(Subject code: 21PGCH13)

Semester: I	Course: 3	Hours/W: 5	Credits: 5

COURSE OUTCOME:

As the course concludes the student will acquire the knowledge and able to

CO1: grasp and correlate the fundamentals of thermodynamics and properties (K2)
CO2: comprehend the knowledge of chemical and physical equilibrium and develop ideas on equilibrium reactions (K3)
CO3: understand the various terms, mathematical operations in quantum chemistry (K1)
CO4: identify the significance of Schrödinger wave equation and its applications (K3)
CO4: develop idea on probability distribution function of electrons (K2)
CO5: evaluate thermodynamic quantities that relate to the inter and intra phase equilibria (K5)
CO6: create skills for problem solving in mechanics of chemistry (K6)

UNIT I Basic Concepts of Thermodynamics 15hrs

Introduction to classical thermodynamics

Partial molar properties – definition, physical significance – general methods of determination – Partial molar volume.Chemical potential – Gibbs Duhem equation – chemical potential of ideal gas and mixture of gases – variation with (i) temperature and (ii) pressure.Fugacity – definition and method of determination in real gases – variation with temperature, pressure and composition (DuhemMargules equation equation) – fugacity of solids, liquids and mixture of real gases – Lewis Randall rule.

Activity concept of condensed states – activity and activity coefficient – choice of standard states – methods of determination for non – electrolytes.Third law of thermodynamic - Planck and Lewis Randall formulations – unattainablity of absolute zero – calculation of absolute entropies – exceptions to third law.

Self study:Hess's law, Henry's law, Richard's law, Vant't Hoff reaction isotherm & isochore

UNIT II: Chemical Equilibria and Physical Equlibria 15hrs

Chemical equlibria - Reaction Gibbs energy, reaction potential, reaction isotherm and direction of spontaneous reactions.Temperature coefficient of reaction Gibbs energy and equilibrium constant(K)

Thermodynamics of irreversible processes: Simple examples of irreversible processes – General theory of near equilibrium processes – Entropy production from heat flow, matter flow and current flow – generalized equation for entropy production – Phenomenological relations –Onsager reciprocity relations, validity, verification - Application of irreversible thermodynamics to thermal diffusion, thermoosmosis, thermo molecular pressure difference.Phase equilibria in three component systems -Three liquid components forming one, two, three pairs of partially.miscible liquids with examples.Two solids and water

systems involving (i) no chemical combination (ii) formation of a double salt (iii) formation of a hydrate by one salt.

Self-study:Coupled flow

UNIT III: Quantum Chemistry I **15hrs**

Dual nature of electrons -De-broglie hypothesis-Concept of wave velocity and group velocity-velocity of debroglie-Bohr's quantization of angular momentum and its application to hydrogen atom. Postulates of classical mechanics – dynamical variables – Newtonian equations– Lagrangian equation – conservative laws.Inadequacy of classical physics with regard to (i) black - body radiation (ii) photoelectric effect. Mathematics of quantum mechanics – Wave function – eigenfunctions and eigenvalues – orthogonality and normalization.Schrodinger time independent wave equation, Postulates of quantum mechanics different types of functions – different types of operators. – commutation relationship among L_x, L_y, L_z and L^2 operators. Wave function – eigenfunctions and eigenvalues – orthogonality and normalization.Schrodinger time independent wave equation, Postulates of quantum mechanics.

Self-study:Transition probability

UNIT IV: Quantum Chemistry II **15hrs**

Setting up Schrodinger equation, solution & interpretation with regard to particle in a 1 –D box, particle in a 3 – D box, electron in a ring, rigid rotor and simple harmonic oscillator & 3 – D uncoupled isotropic oscillator. Setting up Schrodinger equation for H – atom, separation into three equations (without derivation), quantum numbers and their importance – hydrogenic wave functions – analytical and graphical representations – radical probability distribution function

Self-study:Wave function for a free particle & Tunnel effect

UNIT V: Statistical Thermodynamics **15hrs**

Aim – concept of distribution, thermodynamic probability and most probable distribution.S.M. of ensembles – meaning of ensembles – canonical, grand canonical and micro canonical ensembles.Boltzmann distribution law – concept of partition function and its significances. Relation between Partition Functions and thermodynamic functions – illustrative examples– Sackur-Tetrode equation.

Evaluation of independent molecular Partition Functions (translational, rotational, vibrational and electronic partition function) of diatomic & simple polyatomic molecules.Heat capacities of solids – Einstein model and Debye modification. Quantum statistics – Fermi Dirac and Bose Einstein

Population inversion and negative Kelvin temperature – Behavior of Helium at low temperature.Partition function and equilibrium constant.Statistical meaning of third law of thermodynamics

Self-study:Bose-Einstein statistics for Photon gas

REFERENCES

UNIT I

1. J.Rajaram and J.C. Kruiacose – Thermodynamics 2002, Shoban Lal and Co.
2. S.Glasstone – Thermodynamics for chemists, 1947, East West Press.

UNIT II

1. Samuel H. Maron and Carl F.Prutton – Principles of Physical chemistry, 4th ed 1965, Oxford & IBH Publishing Co.Pvt.Ltd.
2. S.Glasstone – A textbook of physical chemistry, 2nd ed., 1969, Macmillian and Co Ltd.

UNITS III & IV

1. A.K. Chandra – Introductory quantum chemistry, 4th ed., 2001 reprint, Tata Mc Graw- Hill.
2. Donald A McQuarrie – Quantum Chemistry, Indian edition, Viva Books Pvt, Ltd.
3. Ira N.Levine – Quantum chemistry, 4th ed (1991), Prentice Hall of India.
4. Peter Atkins, Julio de Paula – Atkins' physical chemistry, 7th ed., 2002, Oxford University Press.
5. J.E. House, Fundamentals of quantum chemistry, 2nd ed., Academic Press, Indian Reprint 2008.

UNIT V

1. Walter J. Moore – Basic physical chemistry, 1986, Prentice Hall Inc, Orient Longman Limited.
2. M.C. Gupta – Statistical thermodynamic, 2nd ed (1988), New age international (p) Ltd.
3. J.Rajaram and J.C. Kruiacose – Thermodynamics for students of chemistry, 2002, Shoban Lal and Co.
4. Peter Atkins, Jutio de Paula – Atkins' physical chemistry, 7th ed., 2002, Oxford University Press.

SELECTED TOPICS IN INORGANIC AND SUPRAMOLECULAR CHEMISTRY

(Subject code: 21PGCHE11)

Semester:I	Elective-1	Hours/W:5	Credits:5

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1: differentiate the use of orbitals in bondings (K2)

CO 2: apply the significance of Inorganic metals as medicine in day -to-day life(K3)

CO 3:analyze the biological functions ofmetals and non-metals in Living system(K4)

CO 4: define supramolecular chemistry, molecular recognition and host-guest chemistry(K1)

CO 5: demonstrate the host-guest assembly in new giant molecules(K3)

CO 6: Summarize the use of dendrimers, supramolecular electronic devices in various fields(K5)

Unit- I: Periodicity and Inter &pseudo halogen compounds 15hrs

First and Second row anomalies, The Use of **p**orbitals in Pi bonding,The Use (or not) of **d** Orbitals by Non-metals, Reactivity and **d**orbital participation, Periodic anomalies of the Non-metals and post transition metals,Halogens in positive oxidation states,Interhalogen compounds, Polyhalide ions,Fluorine-Oxygen chemistry, Halogen cations,Pseudohalogens. Electrochemistry of halogens and Pseudohalogens

Self-Study:Frost Diagram

Unit- II: Biochemistry of metals and non-metals 15hrs

Biochemistry of Calcium,Bio minerals of calcium- calcite, Apatite and Fluorapatite,Storage of calcium, Transport of calcium- calmodulin, Role of calcium in muscle contraction, Role of calcium in blood clotting, Biochemistry of Iron,Transport of Iron- Transferrin, Siderophores, Storage of Iron- Ferritin, Ion transport Mechanism- Na^+/K^+ pump, Biological importance of nitric oxide.

Self-Study:Zinc in transcription

Unit III: Inorganic chemistry in Medicine 15hrs

Ionophore Antibiotics-Valinomycin,Cancer treatment-cisplatin and other Inorganic complexes,Anti-Arthritis drug-Gold, Gastric Ulcer treatment-Bismuth,Mental disorder-Lithium,Malaria treatment-Organometallic drug,Anti-HIV agents-cyclams,Post-operative stress releasing agent,Chelation therapy,Imaging Agents and MRI

Self-Study:The glucose sensor- an application of ferrocene

Unit IV: Supramolecular Chemistry 15hrs

Definition and development of Supramolecular chemistry,Supramolecular chemistry,Host-Guest chemistry,Development of Supramolecular chemistry,concepts of Lock and key interactions, Host-Guest chemistry, and self- assembly,Nature of Supramolecular interactions,Supramolecular chemistry of fullerenes, Fullerene as Host and guest. Role of crown ethers, podands, cryptands,spherands, calixarenes, and siderophores in Supramolecular chemistry

Self-Study:Cyclodextrin

Unit- V: Supramolecular Assemblies and devices 15hrs

Molecular self-Assembly-Catenanes, Rotaxanes and pseudo Rotaxanes.Statistical approaches to Catenanes and Rotaxanes.Catenanes from (pi- pi) stacking interactions. Dendrimers - Synthetic methodology – Divergent and convergent methodologies. Dendrimer Host- Guest chemistry,Dendritic photochemical devices. Molecular electronic devices, Molecular wire, Molecular rectifier,Molecular switch-1,2-dithienyl system.

Self study: Allosteric switch

REFERENCES:

1. 1.James E. Huheey, Inorganic Chemistry, Principles of structure and reactivity,4th edition, Pearson education.
2. Shriver and Atkins, Inorganic Chemistry, 5th edition, Oxford University Press
3. Mark Weller, Tina Overton, Jonathan Rourke and Fraser Armstrong, Inorganic chemistry, 6th edition, Oxford University Press
4. AsimK.Das, Bioinorganic chemistry, Books and Allied (p) Ltd.
5. J.M.Lehn, Supramolecular Chemistry, Concepts and perspectives, 1995, VCH; Weinhein.
6. J.W. Steed, J.L. Atwood, Supramolecular chemistry, 2000, John Willey&sons Ltd. New York.

CORE –PHYSICAL CHEMISTRY PRACTICAL – I

(Subject code: 21PGCHP11)

Semester: I	Practical: 1	Hours/W: 4	Credits: 2

COURSE OUTCOMES:

As the course concludes the student will acquire the knowledge and able to

CO1: Develop practical skills in conductometric and potentiometric titration experiments
CO2: understanding ofthe calibration and use simple instruments intheir experiments
CO 3:design and carry out scientific experiments as well as accurately record and analyze the results of such experiments
CO4: understanding ofthe calibration and use simple instruments intheir experiments
CO5: Are able to identify and solve chemical problems and explore new areas of research

CONDUCTIVITY EXPERIMENTS:

Determinations of

1. a) Strengths of strong acid and weak acid in a mixture or
   b) Strengths of HCl and NH_4Cl in a mixture
2. Strengths of NaOH and CH_3COONa in a mixture
3. Strengths of CH_3COONa and CH_3COOH in an acetate buffer.
4. Strengths of chloride and iodide in a mixture
5. Solubility and solubility product (K_{sp}) of $PbCl_2$, $BaSO_4$ or AgCl.
6. Hydrolysis constant of aniline hydrochloride.
7. The degree of dissociation and equilibrium constant of KCl/acetic acid in different solvents (dioxane, water) andin their mixture; and to test the validity of Debye Huckel Onsager theory.
8. Kinetic-Saponification of ester: Determination of activation energy by conductometry.
9. Determination of critical micelle concentration of Sodium lauryl sulphate (Conductivity method)

POTENTIOMETRIC EXPERIMENTS:

Determinations of

1. a) Strengths of strong acid and weak acid in a mixture or b) Strength of KCl
2. Strengths of Fe^{2+} using $K_2Cr_2O_7$ or ceric sulphate or ceric

ammonium sulphate.

3. pH of citric acid – disodium hydrogen phosphate buffer
4. Strengths of chloride and iodide in a mixture.
5. Solubility product of AgCl, AgBr, $Ag_2C_2O_4$ or Ag_2CrO_4
6. Hydrolysis constant of aniline hydrochloride
7. Dissociation constant of acetic acid in dioxane and water by titrating it with KOH
8. Determination of formation constant of Silver – ammonia complex (Potentiometry)

REFERENCES

1. Dr.K.Karunakaran, Laboratory manual in physical chemistry.
2. V.D. Athawale and Parul Mathur, Experimental physical chemistry, New Age international publishers, 2001.
3. Lab manual supplied by the department

NOTE

Students should submit their record note for evaluation at the time of examination.

Viva voce examination on practicalswill be conducted.

CORE – ORGANIC CHEMISTRY PRACTICAL – I

(Subject code: 21PGCHP12)

Semester: I	Practical: 2	Hours/W: 2	Credit:1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: separate the mixture of organic compounds in microscale (K2)
CO2: apply separation methods to isolate mixtures (K3)
CO3: analyze the organic compounds for functional group (K4)
CO4: determine the melting points / boiling points using digital apparatus (K5)

QUALITATIVE ANALYSIS OF ORGANIC COMPOUNDS (MICRO ANALYSIS)

(i) Pilot separation of organic mixture

(ii) Bulk separation

(iii) Analysis of organic compounds

(iv) Preparation of a solid derivative

(v) Determination of Melting (or) Boiling points of (a) the compounds and (b) any one of the solid derivatives.

REFERENCES:

1. Furniss, Hannaford, Smith, Tatchell.; *Vogel's Text Book Of Practical Organic Chemistry.*, Pearson Education.
2. Bhutani.S.P, ArunaChhikara.; *Practical Organic Chemistry*., Ane books India.
3. Gnanapragasam.N.S., Ramamurthy.G.; *Organic Chemistry Lab Manual*., S.ViswananathanPvt.Ltd.
4. Ahluwalia.V.K, Sunitha Dhingra, Adharsh Gulati.; *College Practical Chemistry.,* University Press.

Note: Students should submit their record note for evaluation at the time of examination.

Viva – Voce examination on practicals will be conducted.

CORE – PRACTICAL ORGANIC CHEMISTRY – II

(Subject code: 21PGCHP13)

Semester: I	Practical: 3	Hours/W: 2	Credit:1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1: describe the procedures to prepare new compounds (K2)
CO 2: experiment the idea into synthesis of organic compounds (K3)
CO 3: Generate new methods to synthesize organic compounds (K6)
CO 4: develop skill in crystallization technique (K6)

PREPARATION OF ORGANIC COMPOUNDS (SINGLE STAGE)

(i) Oxidation of toluene to benzoic acid

(ii) S-Benzylisothiouronium chloride

(i) Bromination of Acetanilide

(iv) Nitration of phenol

(v) Glucosazone

(vi) Methyl orange dye

(vii) Bromination of β - naphthol

REFERENCES:

1. Furniss, Hannaford, Smith, Tatchell.; *Vogel's Text Book Of Practical Organic Chemistry.,* Pearson Education.
2. Bhutani.S.P, ArunaChhikara.; *Practical Organic Chemistry*., Ane books India.
3. Gnanapragasam.N.S., Ramamurthy.G.; *Organic Chemistry Lab Manual*., S.ViswananathanPvt.Ltd.
4. Ahluwalia.V.K, Sunitha Dhingra, Adharsh Gulati.; *College Practical Chemistry.,* University Press.

Note:

Students should submit their record note for evaluation at the time of examination.

Viva Voce examination on practicals will be conducted.

CORE – ORGANIC CHEMISTRY – II (THEORY)

(Subject code: 21PGCH21)

Semester: II	**Core:4**	**Hours/W: 5**	**Credits: 5**

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: state the essential concepts of reaction mechanism, electrophilic substitution, molecular rearrangements, photochemistry and pericyclic reactions (K2)

CO2: illustrate the mechanism of molecular rearrangements and photochemical reactions in organic chemistry (K2)

CO3: apply retrosynthetic approach towards the synthesis of organic compounds (K3)

CO4: analyze the pericyclic reactions using symmetry properties (K4)

CO5: recommend the mechanism for naming reactions (K5)

Unit I Electrophilic Substitution and Elimination Reactions **15 hrs**

Electrophilic substitution at saturated carbon atom, S_E1, S_E2, S_Ei mechanisms, isoinversion,Conducted tour mechanism,Stork enamine reaction,Aromatic Electrophilic substitution reaction,Mechanism of nitration, Friedel Craft alkylation, Acylation reactions,Elimination reactions, E1,E2,E1cB mechanisms, Bredt's rule,Hofmann rule - Saytzeff rule – pyrolytic elimination,Chugaev reaction,Cope reactions

Self-Study:Woodward Prevost hydroxylation

Unit II Organic Photochemistry **15 hrs**

Organic photochemistry -Basic principle-Beer-Lambert's law-Stark Einstein law-Grothus Draper's law-Quantum yield-Classifications of reactions based on quantum yield-Norrish type I and type II reactions, Paterno – Buchi reaction. Photo reduction of ketones - Photochemistry of olefins,Cis-trans isomerisation, Photosensitization - Di –π- methane rearrangement, Photo oxidation-Barton reaction. Photoaddition-Photoaddition of alkene to carbonyl compounds-Photoaddition of alkenes and alkynes to aromatic compounds-Photodimerization of alkene. Photolysis of diazo-compounds, Photochemistry of alpha, beta unsaturated compounds.

Self Study:Photochemistry of arenes.

UNIT III Pericyclic Reaction **15 hrs**

Pericyclic reactions - Molecular orbital symmetry; frontier orbitals of ethylene,1,3-butadiene,1,3,5- hexatriene and allyl system. Classification of pericyclic reactionsWoodward-Hoffmann correlation diagrams. FMO and transition state aromaticity approach-selection rules.Electrocyclic reactions- conrotatory and disrotatory motions; 4n and 4n+2 system. Cycloaddition reactions: suprafacial and antara facial additions; 4n and 4n+2 system. Sigmatropic reactions - Woodward-Hofmann rule and FMO method - Suprafacial and antara facial shifts of Hydrogen - Sigmatropic shifts inoving carbon moieties. 1,3-,1,5- and 3,3-sigmatopic rearrangements. Cope and Claisen rearrangements, Correlation diagram approach

to simple systems. Dis and conrotatory ring closure of 1,3-butadiene, 1,3,5-hexatriene and $\pi^{2s}+\pi^{2s}$ and $\pi^{4s}+\pi^{2s}$ cycloaddition reactions.

Self-Study: Aza-cope rearrangement

Unit IV Retrosynthetic Analysis **15 hrs**

Planning of synthesis - Disconnection approach, Synthons and synthetic equivalents, Synthon Approach-Nucleophiles and electrophiles. Introduction of functional groups, Functional group interconversions. Use of activating and blocking groups in synthesis. One group disconnection: alcohol, olefin, ketone, acids. Two group disconnections: 1,2-, 1,3-, 1,4- and 1,5- difunctional compounds. Convergent Synthesis. Functional group addition

Self-Study:retrosynthetic analysis of multistriatin, synthesis of cubane.

Unit-V Important Synthetic Organic Name Reactions-I **15 hrs**

Jones Oxidation, Dakin reaction, Bouveault –Blanc eaction, Bamford Stevens reaction, Doebner Miller synthesis, Mukaiyama reaction, Pechmann Condensation,Ritter reaction, Sarett Oxidation, Thorpe reaction, Swern Oxidation, Suzuki and Mitsunobu reaction.

Self Study: pd Catalysed coupling reactions

REFERENCES:

1. Francis A.Carey and Richard J.Sundberg, "Advanced Organic Chemistry", 4th Edition, Kluwer Academic Puplishers
2. Clayden, Greeves, Warren and Wothers", Organic Chemistry", Oxford University Press
3. Staurt Warren, "Organic Synthesis 'The Disconnection Approach', John Wiley student edition.
4. William Carruthers and Lain Coldham, "Modern methods of Organic Synthesis", 4th Edition 2004.
5. R.T.Morrison and R.N.Boyd, "Organic Chemistry", 2nd Edition, Prentice Hall
6. I.L. Finar, Organic Chemistry, Vol. I& II, 3rdIndian Reprint, 2001, Pearson Education.
7. R.O.C. Norman, Organic Synthesis, 2nded.
8. V.K.Ahluwalia, RakeshkumarOrganic reaction mechanisms, IV edtion, Parashar ,Narosa Publishing House

INORGANIC CHEMISTRY – II

(Subject code: 21PGCH22)

Semester:II	Core: 5	Hours/W: 5	Credits: 5

COURSE OUTCOME:

By the end of the Course the student will be able to

CO 1: compare and contrast the characters of transition and inner transition elements (K5)
CO 2: describe the theories of coordination complexes (K2)
CO 3: Summarize the idea of kinetics of the complexes (K2)

CO 4: Outline the structural features of inorganic chains, rings and cage compounds (K4)

CO 5: Examine the laws of photochemistry and analyze photochemical behavior of inorganic complexes (K4)

CO 6: recognize the scope of nuclear reactions which brings innovations in future (K5)

Unit-I Transition Elements and Inner transition Elements 15hrs

Transition elements- Electronic structure - General characteristics - atomic, ionic radii – variationalong the period and group.Variable valency, colour, magnetic properties,non-stoichiometric, catalytic property and complexing tendency- Comparison of 1^{st} row with other two rows of transition elements. Stabilizationof unusual oxidation states.Inner transition elements - position in the periodic table – electronicconfiguration, oxidation states, colour and spectra,magneticproperties. Separation of lanthanides –Valency change and Ion exchange method,Lanthanide contraction-Cause andconsequences, Gadolinium break, shift reagents, Comparison of actinides and lanthanides

Self-study: geological survey of lanthanides and actinides

Unit II: Theories of Coordination Chemistry 15 hrs

Qualitative aspects of VB theory. Crystal field theory - Splitting pattern of octahedral, tetrahedral, square planar symmetry. Factors affecting the magnitude of Δ. Magnetic properties, CFSE, high spin-low spin cross over – limitations. Jahn - Teller effect (static,dynamic, elongation and flattening). Ligand Field theory - Evidences for M-L overlap-Nephelauxetic effect. Molecular Orbital theory of octahedral complexes(sigma and pi bonding). MO of tetrahedral and square planar complexes.

Self-study: Information about a complex usingphotoelectron spectroscopy

Unit III: Reaction Kinetics in Coordination Chemistry 15 hrs

Substitution reactions - Substitution reactions in square planar complexes-Mechanism,Trans effect,Trans series, Theories – polarization and pi bonding theory,Applications of trans effect. Substitution reactions in octahedral complexes-Mechanism - Anation reaction and Water exchange reactions.Electron transfer reactions–Inner-sphere mechanism–Outer-sphere mechanisms. Complementary, non-complementary reactions

Self-study: Stereochemistry and isomerization of complexes

Unit- IV: Inorganic chains, rings, cages and clusters 15hrs

Silicate minerals, Classification of silicates, Ortho, pyro, and cyclic silicates – pyroxene, amphiboles. Two dimensional silicates – talc, mica. 3D- silicates- feldspar, zeolites, and ultramarines. Iso and hetero-polyacids-structure of $[TeMo_6O_{24}]^{6-}$ and $[Mo_7O_{24}]^{6-}$ ions. Sulphur nitride – S_4N_4 and polymeric sulphur nitride. Borazine –preparation, structure and properties.Phosphazenes - trimers and tetramers,Concept of multi-centered bond structure of B_2H_6,B_4H_{10},$B_{12}H_{12}^{2-}$,B_6H_{10},B_8H_{12},$B_{10}H_{14}$. Closo, nido, arachnoboranes and carboranes, Metal clusters- $Re_2Cl_8^{2-}$, $Nb_6Cl_{12}^{2+}$, $Mo_6Br_8^{4+}$

Self-study: Polyatomic zintl anions and cations and Chevrel phases

Unit-V: Inorganic photochemistry and Nuclear chemistry 15hrs

Basic laws of photochemistry-Photochemistry of transition metal complexes-photoredox, photo substitution and photoexchange reactions-light induced isomerization, dissociation and linkage isomerization. Photochemistry of Cr and Rupolypyridyl complexes. Photochemical conversion. Ruthenium bipyridyl complexes-splitting of water

Nuclear fission – Characteristics of fission reactions. Fissile and fertile isotopes.Nuclear fusion – Stellar energy, spallation and fragmentation. Nuclear waste disposal - Reprocessing of nuclear materials,Neutron activation analysis, isotope dilution analysis, Theories of alpha and beta decay.

Self-study: Applications of Shell model-Nordheim's Rules

REFERENCES

1. James E. Huheey, Inorganic Chemistry, Principles of structure and reactivity, 4th edition, Pearson education.
2. J.D.Lee, Concise Inorganic Chemistry, 5th edition, 1996, Blackwell science Ltd.
3. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 3rd edition, Pearson education.
4. Miessler and Tarr, Inorganic Chemistry, 3rd edition, Pearson education
5. Shriver and Atkins, Inorganic Chemistry, 5th edition, Oxford University Press
6. Rohatgi and Mukherjee, Fundamentals of Photochemistry, 1986, New Age international publishers.
7. H.J.Arnikar, Essentials of Nuclear Chemistry, 4th edition, New International Limited.
8. Glasstone,S.," Source book on Atomic Energy", 3rd edition, van Nostrand Reinhold Company, 1967 New York.

CORE – PHYSICAL CHEMISTRY – II (THEORY)
(Subject code: 21PGCH23)

Semester: II	Core: 6	Hours/W: 5	Credits: 5

COURSE OUTCOME:

As the course concludes the student will acquire the knowledge and able to

CO1: analyze and assign the molecules based on mathematical background viz; point groups, sub groups, abelian groups etc; gain profound knowledge on theoretical aspects of molecular spectroscopy (K3)
CO2: able to characterize the molecules using IR and Raman spectroscopic technique (K3)
CO3: acquire the basic principles of vibrational spectroscopy (K2)
CO4: analyze IR bands and Raman lines of molecules (K2)
CO5: associate basic idea on auger electron spectroscopy (K2)
CO6: summarize the theories and principle behind NMR and ESR in compounds (K5)

UNIT I Basic principles of Group Theory 15hrs

Molecular symmetry elements and symmetry operations. Axioms of mathematical group. Molecular symmetry point groups-Point group classifications. Group multiplication table – Abelian, non – Abelian, cyclic and sub groups– conjugacy relation and classes.

Representation of symmetry operations by matrices – representation for the C_{2v}. C_{3v}, and C_{2h} to be worked out explicitly – Reducible and irreducible. representations. The great orthogonality theorem and its consequences without proof.Construction of the character tables C_{2v}, C_{3v} and C_{2h}. Direct product concept and direct product representation

Self-study:Huckel Approximation

UNIT II: Application of group theory to spectroscopy and molecular problems 15hrs

Standard reduction formula, Group Theory (GT) applied to determine hybridization scheme in CH_4 and BF_3. Symmetry of normal modes of vibration in$[PtCl_4]^{2-}$. Symmetry of vibration in linear molecules HCN, C_2H_2., NO_3^-ions. Application of GT to normal mode analysis$[PtCl_4]^{2-}$ Symmetry properties of integrals and symmetry – based selection rule for vibrational spectra – Identification of IR and Raman active fundamentals. Symmetry in crystals – Hermann-Mauguin symbols. Space groups of crystals – translational elements of Symmetry. Comparision of crystal Symmetry with molecular Symmetry.Symmetry of molecular orbitals and symmetry – based selection rule for electronic transition – prediction of electronic transitions in ethylene and formaldehyde.

Self-study:Symmetry based selection rule for cyclization reactions, Symmetry Adapted Linear Combinations and LCAO of naphthalene

UNIT III: Molecular Spectroscopy – I **15hrs**

Electromagnetic radiation-Introduction-Region-properties

Microwave Spectroscopy: classification of molecules – Hetero diatomic molecules (Rigid rotor model) – selection rule and rotational spectra – effect of isotopic substitution on transition frequencies – Intensities – non rigid rotor – Stark effect

Vibrational spectroscopy

Infra-red spectroscopy –basic principles– Anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy – P,Q,R, branches – Breakdown of Oppenheimer approximation vibration of polyatomic molecules – overtones, hot bands, combination and differences bands –instrumentation – principle of F.T.I.R

Raman Spectroscopy: Raman scattering– structure determination from Raman and IR spectroscopy

Self-study:Coherent Anti-Stokes Raman Spectroscopy (CARS)

UNIT IV: Spectroscopy – II **15hrs**

. Molecular electronic spectroscopy: Electronic spectra of diatomic molecules- vibrational coarse structure, intensity of vibrational – electronic spectra, dissociation energy, dissociation products, rotational fine structure of electronic –vibrational transitions, Fortrat diagram – Birgesponer extrapolation

X-ray Photo electron spectroscopy (XPES) – Basic principles - photoelectric effect, ionization Process - Koopman's theorem – atomic photo electron spectra, photo electon spectra of simple molecules – ESCA and chemical information from ESCA – instrumentation (UVradiation, X-ray photo electron spectrometer) –Auger electron spectroscopy (AES)

Self-study:Debye Scherrer Method

UNIT V: Spectroscopy – III **15hrs**

Proton NMR: Nuclear spin, Nuclear resonance, saturation, interaction between spin and magnetic field, gyromagnetic ratio, Larmor precessional frequency – relaxation processes in NMR – Bloch equations – chemical shift – shielding of magnetic nuclei, measurement of chemical shift, factors affecting chemical shift, Indirect spin – spin interaction and coupling constant (J), Overhauser effect – FTNMR and its advantages.

Electron Spin Resonance (ESR) Spectroscopy: Theory of ESR – positions of ESR adsorptions – electron 'g' value – hyperfine splitting in ESR – zero field splitting, Kramer's rule – Application to electron exchange reactions – calculation of electron density in radicals

Nuclear Quadrupole Resonance (NQR) Spectroscopy – quadrupole nuclei, quadrupole moments, electric field gradient – requirement for observing NQR spectra – quadrupole coupling constant in atoms and molecules – application in determining ionic characters and hybridization – experimental set up. Mossbauer spectroscopy -. Principle, Doppler shift, Recoil energy – Isomer shift – Quadrupole splitting - Hyperfine splitting – applications to various compounds

Self-study:Photoacoustic spectroscopy (PAS) and Optoacoustic spectroscopy (OAS)

REFERENCES

UNITS I & II

1. F.A. Cotton – Chemical applications of group theory, 3rd ed., 1992, A Wiley Interscience publications.
2. V.Ramakrishnan and M.S. Gopinathan – Group theory in chemistry , 2nd ed., 1991, Vishal publishing Co.
3. K.V.Raman – Group theory and its applications to chemistry, 1990, Tata McGraw Hill Publishing Co. Ltd.
4. Bancroft.M. Mossbauer spectroscopy-Tata Mc Graw- Hill Publishing company New Delhi 1978

UNITS III, IV & V

1. C.N. Banwell and E.M. Mc Cash – Fundamentals of molecular spectroscopy, 4th ed., 2002, Tata Mc Graw – Hill Publishing Co. Ltd.
2. B.P. Straughan and S.Walker (Ed) – Spectroscopy Vol. I, II and III, 1976, Chapman and Hall.
3. R.S. Drago – Physical methods in chemistry, 1977, Saunders College Publishing.

ELECTIVE - OPTIONAL I
PHARMACEUTICAL CHEMISTRY
(Subject code: 21PGCHE21)

Semester: II	Elective: 2	Hours/W: 5	Credits : 5

COURSE OUTCOME:

By the end of the Course the student will be able to

CO1: list the sources, synthesis and metabolism of various drugs and clinical chemistry (K1)

CO2:summarize the relation between chemical structure and pharmaceutical activity and suitable drugs for various diseases (K2)

CO3:apply the knowledge gained about the various drugs (K3)

CO4: analyze the usage of drugs in our day-to-day life (K4)

CO 5: Recommend the optimization of drugs and its side effects (K5)

CO 6: explain the mechanism of action and adverse effects of various drugs (K5)

Unit-I Introduction to Chemistry of Drugs **15 Hrs**

Drugs- Sources-Classification (Biological, chemical, commercial and utility), Nomenclature of drugs, Biotransformation, Drug design, Factors affecting the stability of drugs, Encapsulation- Drug delivery systems and sustained release of drugs

Unit-II Pharmaceutical Aids **15 Hrs**

Preservatives, Antioxidants, sequestering agents, Emulsifiers, Colorants, Flavoring agents, Sweeteners, Stabilizers, Suspending agents,Ointment bases, Solvents

Unit-III Common Diseases and Treatment **15 Hrs**

Insect,Air,Water borne diseases, treatment using drugs. Digestive disorders,Nervous disorder and Respiratory disorder and their Treatment– Treatment other common diseases (Ulcer, Vomitting, Pellagra, Goiter, Piles and Leprosy).

Unit-IV Pathogenicidal drugs **15 Hrs**

Antibiotics - Classification- Chloramphenicol, Penicillin, Streptomycin,

Tetracycline,acrolides, Erythromycin, Rifamycin, Antiseptics and disinfectants, Phenols Halogen compounds, Analgesics, Antipyretics, Anti –inflammatory agents, Sulpha drugs

Unit-V Bio regulatory Drugs **15 Hrs**

Cardiovascular drugs - Cardiac glycosides - Anti arrhythmic drugs - Antihypertensive agents

Antianginal agents, Diabetes, Hypoglycemic drugs , Types of diabetes, InsipidusMellitus, Control of diabetes, Insulin, Hypoglycemic agents - Anticonvulsants,Cancer - Antineoplastic drugs, Common Causes, Antimetabolites, Muscle relaxants

REFERENCES:

1. Silverman R B, The Organic Chemistry of Drug Design and Drug Action, Academic Press.
2. Lednicer D, Strategies for Organic Drug Synthesis and Design, John Wiley.
3. William Foye, Principles of Medicinal Chemistry; 4th edition, Lippincott, William and Wilkins.
4. A Kar, Textbook of Medicinal Chemistry, Asian Age Publication.
5. Sriram D and Yogeshwari P, Medicinal Chemistry, Pearson Education.
6. Ahluwalia V K, Chopra Madhu, Medicinal Chemistry, Ane Books India.
7. Jayashree Gosh, Textbook of Pharmaceutical chemistry, 1997, S.Chand& Chand publications, New Delhi.

ELECTIVE - OPTIONAL II

CURRENT TRENDS AND RESEARCH TECHNIQUES IN MEDICINAL CHEMISTRY

(Subject code: 21PGCHE21)

Semester: II	Elective: 2	Hours/W: 5	Credits: 5

By the end of the Course the student will be able to

CO1: define, compare and distinguish the methods involved in drug design (K5)

CO2: Understand the fundamentals on CADD (K1)

CO3: Analyze the Dose response curve in view toxicity and therapeutic value (K3)

CO4: Gain familiarity in full, semi –synthesis and combinatorial chemistry (K1)

CO5: examine the role of chiral molecule in drug design. (K3)

CO6: Compare the basic criteria of *in vitro* and *in vivo* bio assay (K3)

UNIT IMETHODS INVOLVED IN DRUG DELVELOPMENT 15 HRS

Medicinal chemistry – introduction- target identification, target prioritation / validation. Lead identification – lead optimization. Requirement for human trial- Preclinical technology– pharmaceutics,Pharma cology and toxicology. Clinical studies- Phase-1, 2 and 3. Drug approval- Phase IIIb /Phase IV studies – post approval studies.

UNIT IICOMPUTER AIDED DRUG DESIGN - CURRENT TREND 15 HRS

Introduction-CADD methodology, small molecule -based drug design,quantitative structure active relationship, molecular descriptors-Electronic parameters and Hammett 's σ constant. Hydrophobicity descriptors, Steric descriptors, Steric descriptors. Molecular connectivity Index, Topliss approach, Pharmacophore based drug design

UNIT IIIAPPLICATION AND FUTURE PERSPECTIVE OF COMPUTER AIDED DRUG DESIGN 15 HRS

Big data, Webserver, Work flow, Machine learning-application of machine learning in drug desing and deep learning, Artificial Intelligence . Molecular dynamics – General aspects of molecular dynamics, Application of molecular dynamics in drug design.

UNITIVPLANING TOTAL, SEMI AND COMBINATORIAL SYNTHESIS 15HRS

Synthetic considerations- Full synthesis,semi-synthetic syntheses,biosynthesis, chirality and asymmetric centers, Resolution of a chiral alcohol. Combinatorial synthesis – Definitoin parallel synthesis, Solid phase synthesis and Combinatorial libraries.

UNIT VBIOLOGICAL TESTING AND BIOASSAYS 15 HRS

Introduction- Testing - *in vitro* models-Enzyme inhibition- Lineweaver – Burk plot, Receptor studies, Affinity, Efficacy, Microbiological testing, High throughput screening, Testing by NMR spectroscopy. Testing - *in vivo* models – Test systems, drug potency, Therapeutic Index- therapeutic dose and lethal dose curves.

REFERENCES

UNIT I:

1. Sriram D and Yogeshwari P, Medicinal Chemistry, Pearson Education

UNIT II and III

1.Fernando D. Prieto-Martı´nez et al. Computational Drug Design Methods—Current andFuture Perspectives. *Chapter* 2, 19-24,2019. doi no:10.1016/B978-0-12-816125-8.00002-X

2.Sriram D and Yogeshwari P, Medicinal Chemistry, Pearson Education

UNIT IV and V

1. Graham Patrick, Medicinal Chemistry, Garland Science Taylor and Francis Group. Special India Edition, 2001

CORE – PHYSICAL CHEMISTRY PRACTICAL – II
(Subject code: 21PGCHP21)

Semester: II	Practical: 4	Hours/W: 4	Credit: 2

By the end of the Course the student will be able to

CO 1: Are able to communicate the results of their work to chemists and non-chemists

CO 2:expertise in the applied concepts of kinetics, thermodynamics and adsorption

CO3:Develop problem-solving & troubleshooting ability in experimental physical chemistry

CO 4:Understand experimental knowledge on kinetics and surface chemistry

CO 5: design and perform experiments to determine the rate, order, and activation energy of chemical reactions by varying concentrations and/or temperature

1. Study of phase equilibria involving formation of a compound with congruent melting point and determination of composition of test mixture. (or) Construction of phase diagram of $CHCl_3$ – acetic acid – water system.
2. Determination of association factor, distribution constant, association constant, and mass of benzoic acid distributed between benzene and water.
3. Study of phase diagram of two compound forming a simple Eutectic
4. Determination of acetic and basic dissociation constant of an amino acid (Glycine) and hence its isoelectric point (pH – metry) (or) Determination of Hammett constant of o-, m-, p- amino / nitro benzoic acid (pH – metry)
5. Determination of kinetic order w.r.t.I^- and w.r.to $S_2O_8^{2-}$ and determination of $[I^-]$ and $[S_2O_8^{2-}]$ in the reaction, in solution, between $K_2S_2O_8$ and KI(by studying it as iodine clock reaction) (or)

   Study of the effect of ionic strength of the medium (i.e, primary salt effect on the velocity constant of $S_2O_8^{2-}$ and I^- reaction, the effect of temperature on rate constant and determination of the activation energy.
6. Determination of the rate constant of a reaction between acetone and iodine in the presence of a mineral acid (HCl) or determination of the relative strengths of acids.
7. Determination of strength of oxalic acid or acetic acid from the study of its adsorption on activated charcoal.
8. Determination of limiting viscosity number (Staudinger index) and molecular weight of a polymer by viscosity method. (or) Determination of radius of molecule (e.g. glycerol) by viscosity measurements.
9. Determination of solubility of benzoic acid over a range of temperature and hence heat of solution.

REFERENCES

1 Dr.K.Karunakaran, Laboratory manual in physical chemistry.

2. V.D. Athawale and Parul Mathur, Experimental physical chemistry, 2001 New age international publishers.

3. Lab manual supplied by the department

NOTE

Students should submit their record note for evaluation at the time of examination. Viva voce examination on practicals will be conducted

INORGANIC CHEMISTRY PRACTICAL– I

(Subject code: 21PGCHP22)

Semester: II	Practical:5	Hours/W: 2	Credit:1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: identify the cations into various groups (K2)

CO2: analyze the familiar and less familiar cations in a mixture (K3)

CO3: compare and contrast cations into groups in a mixture (K5)

CO4: integrate the qualitative ideas into the field of industry (K6)

SEMI MICRO QUALITATIVE ANALYSIS

Analysis of salt mixture containing **two familiar and two less familiar cations** from the following metals.Hg, W, Pb, TI, Se, Te, Mo, Cu, Bi, Cd, Sb, Ce, Th, Zr, Ti, V, Cr , Mn, Al, U, Ni, Co, Zn, Mn, Ca, Ba, Sr, Li, Cs and Mg.

Note:

Students should submit their record note for evaluation at the time of examination.

Viva – Voce examination on practical will be conducted.

REFERENCES:

1) G.Svehla, Vogel's Qualitative Inorganic Analysis, 1996, Pearson education Ltd.

2) V.V.Ramanujam, Inorganic semi-micro Qualitative analysis, 3rd edition, 1974, The National Publishing Company.

INORGANIC CHEMISTRY PRACTICAL – II

(Subject code: 21PGCHP23)

Semester: II	Practical:6	Hours/W : 2	Credit : 1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1: recall the principles of complexometric titrations (K1)

CO2: determine the concentration of metal ions by complexometric method (K3)

CO 3: Compare the different quantitative analysis with EDTA titration (K5)

CO 4: generate the ideas on developing new conditions to favor complexometric experiments(K6)

Estimation of a metal ion present in a mixture by EDTA titrations.

1. Ca and Ba (both using different indicators)
2. Cu and Pb (Pb removed as $PbSO_4$)
3. Mg and Ba (Ba removed as $BaSO_4$)
4. Zn and Pb(Pb removed as $PbSO_4$)

Note:

Students should submit their record note for evaluation at the time of examination.

Viva – Voce examination on practical will be conducted.

REFERENCES:

1) J.Mendhem, R.C. Denney, D. Barnes, M.J.k.Thomas, Vogel's Textbook of Quantitative chemical Analysis, 6^{th} edition, 2002, Pearson Education Ltd.

CORE – ORGANIC CHEMISTRY – III (THEORY)

(Subject code: 21PGCH31)

Semester: III	Core: 7	Hours/W: 5	Credits: 5

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1:list out the principles of selection rules for spectroscopic techniques (K2)

CO2: illustrate the applications of UV, IR, NMR and Mass spectroscopic techniques in studyingorganic reactions. (K2)

CO3: assign the molecular rearrangements and propose their mechanism (K3)

CO4: determine the structure of the organic compounds using UV, IR, NMR and Mass spectral techniques (K4)

CO 5: Classify the structures of biomolecules and steroids (K4)

CO 6: Summarize the complete characters of steroids and heterocyclic compounds (K5)

Unit – I Spectroscopy **15 hrs**

Ultra-Violet (UV), Infra-Red Spectroscopy (IR) and ORD. UV: Basic principle – the absorption laws – types of electronic transitions- influence of solvent and H-bonding on λ_{max} values. Woodward-Fischer rules to calculate λ_{max} values of conjugated dienes and αβ – unsaturated ketones and Scott's rule.IR : Basic principle – instrumentation – characteristic of IR absorptions of different functional groups – factors influencing the IR absorption of molecules. Optical rotatory dispersion (ORD): Octant rule and their applications(R+ methyl cyclohexanone and steroidal ketone) α-haloketone rule -Circular dichroism (CD)

Self-Study: cotton curve of (-)trans-2-decalone

Unit II ^{1}H NMR and ^{13}C – NMR Spectroscopy **15 hrs**

^{1}H– NMR spectroscopy, Basic principle- Number of signals- Chemical shift -Factors influencing the chemical shifts - Spin-spin coupling - Coupling constant and factors influencing the coupling constant -Simplification of spectra: Shift reagents, deuterium substituents and spin decoupling.^{13}C-NMR spectroscopy - Basic principle- Comparison with ^{1}H-NMR – noise decoupling – off resonance decoupling - Factors affecting the ^{13}C chemical shifts - Additivity relationship: calculation of chemical shifts of aliphatic hydrocarbons up to five carbon atoms (data must be given),NOE, 2D NMR and 3D NMR- elementary ideas.

Self study:classification of spin systems and analysis of AX, AMAX, ABX

Unit III Mass spectrometry **15 hrs**

Basic principles - Base peak - Molecular ion peak- Metastable peak -Isotopic peak - Nitrogen rule- Determination of molecular formula from isotopic peak- General rules for fragmentation pattern: McLafferty rearrangement. retroDiels-Alder reaction – ortho effect - Fragmentation pattern of simple compounds of hydrocarbons, amines, alcohols, ketones, acids and phenols

Self-Study:Even electron rule, rule of 13 and Stevenson's rule

UNIT IV MOLECULAR REARRANGEMENTS 15 hrs

Introduction- migration, origin, terminus, migratory, aptitudes, memory effects-1,3-alkyl migration- Pinacol rearrangement. 1,2-aryl migroaddition- Benzil–Benzilic acid rearrangements. Carbon to nitrogen migration- Neber Rearrangement via azirine intermediate, Wolf Rearrangement via ketene intermediate, Arndt-Eistert homologation. Nitrogen- migro detachment rearrangements-Curtius, Lossen and Schmidt. Molecular Rearrangement involving concerted mechanism- Fries, favorskii.Tiffenev – Demyanov, Hydroperoxide rearrangement, Beckmann,Fries,Baeyer–Villiger, stevens rearrangement.

Self-Study: Aromatic rearrangement involving intermolecular migration from N-C: N-haloanilides

Unit V Biomolecules and Hetero cyclic Chemistry 15 hrs

Biomolecules – Steroids, Classification – Conformational aspects of A/B cis and A/B trans steroids. Structural elucidation of cholesterol (Synthesis not required). Synthesis of androsterone, testosterone and progesterone Bile acids. Carbazole, oxazole iso oxazole, coumarins, iso coumarins and chromones - synthesis and general reactions.

Self-Study:structure and reactivity of coumarin and isocoumarin

REFERENCES

UNITI & II & III

1. William Kemp – Organic Spectroscopy, Reprint 2005, ELBS.
2. B.M. Silverstein, G. V. Bassler and T.C. Moril – Spectrometric Identification of Organic Compounds, 4th ed. 2002, Wiley.

UNIT IV

1. P.De Mayo, ‘Molecular Rearrangements”
2. Jerry March, “Advanced Organic Chemistry”, Student Wiley 4th edition, Reprint 2003.

UNIT V

1. I.L. Finar, Organic Chemistry, Vol. I &II, 3rdIndian Reprint, 2001, Pearson Education, R.O.C. Norman, Organic Synthesis, 2nded.
2. Thomas.L.Gilchrist, III edition Heterocyclic chemistry
3. Stanely Thornes, III and IV edition Heterocyclic Chemistry
4. J.A.Joule and K.Mills, Heterocyclic Chemistry, Black well publishers.

INORGANIC CHEMISTRY – III

(Subject code: 21PGCH32)

Semester: III	Core- 8	Hours/W: 5	Credits: 5

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1:summarize the concepts of electronic spectra, stability, kinetics of coordination complexesand inorganic complexes in biology (K2)

CO 2: Examine the concepts and structures of organometallic compounds (K3)

CO2: construct Orgel and Tanabe - Sugano diagrams for inorganic complexes (K3)

CO3: analyze the structure, reaction kinetics and mechanism of coordination compounds(K4)

CO5: evaluate the stability and reaction mechanism of the coordination compounds using electron transfer and substitution reactions (K5)

CO 6: justify the biological functions of inorganic macrocyclic complexes in living system (K5)

Unit- I: Organometallic chemistry-I **15hrs**

Metal carbonyls - Structures of $Fe(CO)_5$, $Fe_2(CO)_9$,$Fe_3(CO)_{12}$, $Co_2(CO)_8$, $Mn_2(CO)_{10}$, $Os_4(CO)_{14}$– stability based on EAN rule.Metal nitrosyls – types based on structure.Metal dinitrogen complexes – structure and bonding Metallocenes- Preparation, reactions, structure and bonding of ferrocene. Half sandwiched molecules and piano stool molecules.Other aromatic cyclopolyene complexes. Sigma and pi-hapto nomenclature, Arene complexes, Non – aromatic complexes, Metal-Olefin complexes- Zeise's salt, Metal-acetylene complexes, Metal-Allyl complexes

Self-study: Isolobal analogies

Unit- II: Organometallic chemistry -II **15hrs**

Catalysis involving organometallic compounds, Oxidative addition and reductive elimination, Hydrogen abstraction, Insertion and Elimination reaction, Homogeneous and Heterogeneous catalysis,Hydrogenation of olefins (Wilkinson's catalyst),Hydromethylation (Oxo process),Oxidation of olefins (Wacker process),Polymerization of propylene (Ziegler-Natta catalyst),Cyclo-oligomerization of acetylenes(Reppe's process),Olefin metathesis, Fischer-Tropsch, Carbonylation of alcohols (Monsanto process), Water-Gas Shift reaction**Self-study: Electro catalysis and photo catalysis**

Unit- III: Physical methods in Inorganic chemistry – I **15hrs**

Electronic spectra,Selection Rules-Term symbols, Orgel and Sugano – Tanabe diagrams. Characteristics of electronic spectra of $d^1 – d^9$ metal ions, Spectral properties of Lanthanides and Actinides. charge transfer spectra. Infrared spectra of Coordination complexes - characteristic frequencies-mode of coordination and interpretation of ClO_4^-, SO_4^{2-}, CO_3^{2-}, ester, amine, amide, DMSO and urea using IR spectra.IR spectra for carbonyl complexes.

Self-study: Magnetism of complexes

Unit- IV: Physical methods in Inorganic chemistry-II 15hrs

Nuclear magnetic resonance (NMR). Applications of multiprobe NMR to inorganic compounds- Electron paramagnetic resonance – Hyperfine splitting, g – factor, zero field splitting and Kramer's degeneracy.Applications of EPR in Cu (II) and Mn (II) complexes Mossbauer spectroscopy - principles –Isomer shift–Quadrupole and magnetic interactions in iron and tin complexes. Applications – MB spectroscopy of octahedral high and low spin iron complexes, pi-back coordination in iron complexes and iron carbonyls. MB studies in tin compounds

Self-study: application of structural elucidation using spectroscopic studies

Unit V: BioInorganic Chemistry-I 15hrs

Metalloporphyrins, Chlorophyll, Photo synthetic electron transport sequence, Cytochrome, Iron-sulphur proteins- Rubredoxin and Ferredoxin, Blue Copper proteins, Hemoglobin and myoglobin, Hemerythrin and Hemocyanin. Cyanide and carbon monoxide poisoning, Vitamin-$B_{12,}$ Nitrogen fixation – *In-vitro* and *in-vivo* nitrogen fixation. Metal Complexes-Biocompatibility and activity.

Self-study: Vaska's complex as synthetic oxygen carrier, Iron protein as sensors

REFERENCES:

1. James E. Huheey, Inorganic Chemistry, Principles of structure and reactivity, 4th edition, Pearson Education.
2. F.A.Cotton and G.Wilkinson – Advanced Inorganic Chemistry, 3rd edition, Pearson education.
3. R.S.Drago,"Physical methods in chemistry", 1st edition, W.B. Saunders Company, Philadelphia.
4. E.A.V.Ebsworth – Structural methods in Inorganic chemistry
5. Mark Weller, Tina Overton, Jonathan Rourke and Fraser Armstrong, Inorganic chemistry, 6th edition, Oxford University Press.
6. D.Sutton – Electronic spectroscopy of transition metal complexes, McGraw – Hill.
7. Lippard, Berg, Bertini and Valentine, Bio- inorganic chemistry, University Science Books
8. AsimK.Das, Bioinorganic chemistry, Books and Allied (p) Ltd.
9. R.Gopalan and V. Ramalingam – Concise coordination chemistry, University Science Books.

CORE – PHYSICAL CHEMISTRY – III (THEORY)
(Subject code: 21PGCH33)

Semester: III	Core:9	Hours/W: 5	Credits: 5

COURSE OUTCOMES:

As the course concludes the student will acquire the knowledge and able to

CO1: compare various theories in kinetics for study of reaction mechanics (K3)

CO2: familiarize on Hammett and Taft equations (K2)

CO3: analyze kinetics of various complex and fast reaction (K2)

CO4: understand basic ideas of photochemistry in physical chemistry point of view (K2)

CO5: examine the electrochemical knowledge of molecules and ions (K3)

CO6: understand and explore molecular interactions, kinetics and electrochemical process (K3)

Unit-I- Chemical Kinetics - I **15 Hrs**

The kinetic theory of collisions & weaknesses, Potential energy surfaces (PES)-PES of ($H+H_2$)-reaction coordinate. Conventional transition state theory (CTST)-Eyring equation and its significance-application to reactions between (i) atoms (ii) molecules-thermodynamic formulation of CTST – relation between $\Delta H°$ and E_a.ARRT Statistical and thermodynamic treatment. Elementary reactions in gas phases: Lindemann-Christiansen, Hinshelwood, RRK, Primary and secondary kinetic isotope effects- - explosion and explosion limits (H_2+O_2)- Elementary reactions in solution between ions: influence of ionic strength (i.e., primary and secondary salt effects)and substituents (i.e., Hammett and Taft equations)- Hammett – a linear Gibbs energy relation.

Self-study: Rideal-Eley mechanism

Unit-II – Chemical Kinetics - II **15 Hrs**

Fast reactions: General features-need for special techniques-flow techniques-relaxation. theory and relaxation techniques (T-jump and P-jump) - crossed molecular beam technique.Need for special technique-Chemical relaxation techniques-Pulse radiolysis-Flash Photolysis

Homogeneous catalysis: general catalytic mechanisms(equilibrium treatment and steady state treatment)- general acid- base catalysis and determinination of catalytic coefficients-discussion of protolytic and prototropic mechanisms of acid catalysis – Bronsted relationships as linear Gibbs energy relationships- acidity functions and correlation of mechanisms, Hammette- Zucker hypothesis

Heterogeneous catalysis (i.e., reactions on surfaces): physisorption and chemisorption-Langmuir adsorption isotherm – competitive adsorption – (BET-isotherm-determination of surface area- Gibbs isotherm) mechanisms of surface reactions (Langmuir-Hinshelwood and Eley-Rideal mechanisms)-absolute rates of surface reactions. Enzyme catalysis – Michaelis Menten equation

Self-study:Ortho effect, Swain-Scott Equation & Yukawa-Tsuno Equation

Unit-III-Photochemistry and Radiation Chemistry **15 Hrs**

Photochemistry-Importance-Photochemistry and Spectroscopy-Thermal emission and photo luminescence-Photo excitation-Dipole moment, pK_a and redox potentials of electronically excited state molecules

Jablonski diagram for a molecule with even number of electrons and various photophysical processes- Time constants & approximate first order rate constants- quantum yield of each event Phosphorescence - ϕ^o_F and ϕ^o_P.

Photochemical reactions and its kinetics

Quenching mechanism- Stern-Volmer equation (derivation, limitation and applications)

Delayed fluorescence (E-type & P-type)Energy transfer mechanisms for bimolecular quenching

Photoisomerization, photostationary stateBimolecular photoprocesses: Excimers, exciplexes and sensitization.

Photochemical kinetics of (H_2+Br_2) reaction, PhotosynthesisRadiation chemistry:radiolysis of Fricke dosimeter solution- radiolyis of water – production, detection and reactions of hydrated electron- G-value- uses of radiation chemistry in industries and medical field.

Self-study:Stark Einstein law & Beer Lambert law derivation

Unit-IV-Electrochemistry-I **15 Hrs**

Fundamentals of electrochemistry – Electrochemical cells-two and three electrode system – influence of solvent on ion conductance and Walden rule- abnormal ionic conductances – Debye Huckel theory- Theory of electrolytic conductance: Ionic atmosphere – thickness of ionic atmosphere – Debye-Huckel theory for conductivity – Debye-Huckel – Onsager conductance equation (derivation, verification and modification) – conductance at high frequencies (Debye-Falkenhagen effect) – conductance at high potential gradients (Wien effect)Activity and activity coefficient –– The Debye-Huckel limiting law (DHLL)–DH equation for appreciable concentrations- The Huckel and Bronsted equations – The Osmotic coefficient – Activities at appreciable concentrations and in concentrated solutions – ion association.

Self-study: Bjerrum model

Unit-V-Electrochemistry-II (Electrode Processes) **15 Hrs**

Significance of electrode-electrolyte interface - formation of electrical double layer (EDL)-contributions to the total potential difference- concept of surface exess- electrocapillarity, electrocapillary curves, Lippmann equation of electrocapillarity , Lippmann potential and measurement.

Structure of electrified interfaces: Double layer - Helmholtz-Perrin, Gouy-Chapman and Stern models – their applications and limitations.

Electrode kinetics-mechanism of electrode reaction rates of one electron electrode reactions-Butler-Volmer (BV) equation-high field and low field approximations-Nernst equation as a special case of BV equation- charge transfer resistance and differential resistance- empirical Tafel equation.

Electrokinetic phenomena: Electroosmosis and electrophoresis- determination of zeta potentials

Principles and working of cyclic voltammetry, Electrochemical applications in energy (primary cells, storage batteries, fuel cells)

Self-study: EMF of the Concentration Cell with Liquid junction potential

REFERENCES:

1. K.J. Laidler, 'Chemical kinetics", 3rdedn. Low Price edn., 3rd Impression, 2009, Pearson Education,
2. J. N. Bradley, "Fast reactions" 1975, Clarendon Press, Oxford.
3. K.K. Rohatge – Mukherjee, "Fundamentals of photochemistry", 1986, Wiley Eastern Ltd.,
4. G. Hughes, "Radiation Chemistry", Oxford Chemistry Series.
5. S. Glasstone, "An introduction to electrochemistry", 1942, East – West Press.
6. D.R. Crow, " Principles and applications of electrochemistry", 2nd Edition, 1984, Chapman and Hall.
7. W.J. Moore, "Physical Chemistry", 4th edition, 1965, Longmans.
8. P.Atkins, Julio de Paula, Atkins's Physical Chemistry, 7th ed, 2002, Oxford University Press.
9. A.J. Bard, Electroanalytical Techniques
10. J.O. Bockris& Reddy, Modern Electrochemistry, Vol. I, II & III.

ELECTIVE - III
RESEARCH METHODOLOGY (Theory)
(For Internal evaluation only)
(Subject code: 21PGCHE31)

Semester: III	Elective:3	Hours/W: 5	Credits: 5

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: Develop scientific temper in understanding a problem (K3)

CO2: Exposed to scientific literature and able to grasp current scientific knowledge (K2)

CO3: Examine a research problem and find a suitable to solution for the same (K5)

CO4: grasp idea on statistical tools in processing the experimental data acquired (K2)

CO5: develop a skill of writing scientific report; interpret the results of a scientific study (K5)

CO6: Inculcate Oratory Skills with visual aids in participating scientific gathering.(K5)

UNIT 1 Introduction to research approaches 15 hrs

Definition of research, Defining the research problem, need for surveying scientific literature. Scientific method, Criteria for good research and significance, Types of research – Fundamental, applied and mixed research, Hypothesis testing- Null and alternate hypothesis, Research via scientific methods.

Unit-II Literature survey 15 hrs

Primary sources-journals and patents,Secondary sources-listing of titles, Beilstein, Compedia, tablets of information, reviews, monographs and text books,Literature searching-information about a specific compound, science citation index and locating journals (articles), information retrievals with internet. Research paper format in Journal of American Chemical Society, Journal of Chemical Society, RSC,Wiley,Springer link and Tetrahedron. Indepth study of two papers from any leading international journals

Unit-III Methods of reporting computed data

Types of errors, Accuracy, Precision, Significant figures, Frequency distribution, Binomial distributions, Poisson distribution, Normal distribution, Different methods to reduce systematic errors, Mean and standard deviation, Q-test, student's *t*-test, paired *t* test, and F-test and outlier detection,Analysis of Variance (ANOVA). LSM of finding the best straight line, Assymetric deviation (mean, median and mode),Errors in the slope and intercept.

UNIT IV Computer in research 15 hrs

Chemdraw – drawing, chemical structure- chemdraw basics- starting chemdraw-working with document-drawing chemical structures-3D structures- energy minimization-viewing3D molecules-molecular dimensions-molecular properties-partial charges-molecular electrostatic potentials-molecular orbitals-spectroscopic transitions-local and global energy minima-molecular dynamics-stepwise bond rotation-automated screening of databases for lead molecules- Introduction to SPSS- Data view, variable view, Descriptive statistics, Compare means- ANNOVA (one sample and two sample t tests) and cart builder. Molecular docking – docking procedures – manual docking – automatic docking using docking softwares.

Unit-V Report writing and oral presentation 15 hrs

Interpretation- Meaning, Technique, precaution- Significance of Report writing and precautions- Layout of the research report. Thesis layout - Format of title page, certificates, declaration, preface, acknowledgements and table of contents - Text of the thesis: Use of centered heading, side heading and paragraph heading- Quotations: the ways to use quotations, interpolation of quotations, Footnotes.

Tables and Figures: format, conventions and referencing- Documentation: methodology of writing references - Editing and evaluating: Basic idea of editing, revising and evaluating the thesis

. The oral presentation - proactive research preparation, achieving focus, organizing the presentation, using language effectively, achieving speaking excellence and visual aids

REFERENCES

1. March, J., Advanced Organic Chemistry (Appendix A), Fourth Edition, 2000, John Wiley & Sons, New Delhi.
2. Kothari.C.R., Research methodology methods and techniques, second edition,1990, New age international (P) Limited, New Delhi, India.
3. Abdul Rahim, F., Thesis Writing – A Manual for Researchers, 1996, New Age International Ltd., New Delhi.
4. Laurie, R., Guide to Writing Great Research Papers, 1999, McGraw Hill, New York.
5. Skoog, D.A. West, D.M., Holler, F. J. and Crouch, S.R., 2004, Fundamental of Analytical Chemistry, Thomson, Eighth Edition, Singapore.
6. Willard, H. H., Merrit, L.L., Dean, F. A. and Settle, J. A., 2006, Instrumental Methods of Analysis, CBS Publishers, Seventh Edition, New Delhi.
7. Mendham, J., Denney, R.C., Barenes, J.D. and Thomas, M.J.K., 2004, Vogel's Text Book of Quantitative Chemical Analysis, Sixth edition, Pearsons Education, New Delhi.
8. Fujita, H., Micromachines as Tool for Nanotechnology, 2003, Springer-Verlag Berlin Heilderberg, Chapters 5 and 8.
9. Cao, G. Nanaostructres and nanomaterials – Synthesis, Properties and Applications, 2004, Imperial College Press, London, Chapter 7.
10. Alexis, L. and Mathews, L., Fundamentals of Information Technology, 1999, Leon Vikas, Chenna

ELECTIVE – III
CHEMINFORMATICS
(For Internal evaluation only)
(Subject code: 21PGCHE31)

Semester: III	**Elective:3**	**Hours/W: 5**	**Credits: 5**

Course Outcomes

On successful completion of the course, the learners should be able to
CO1[K2]: understand the principles of cheminformatics
CO2[K3]: predict the bioactivity using structure and evolutionary relationship
CO3[K3]:apply 2D, 3D structure in the evaluation of similarity method, 3D pharmacophore investigation and drug designing process.
CO4[K4]: realize the importance of data base, sequence analysis, QSAR and docking in the drug discovery process
CO5[K5]:discuss data base, structure analysis, sequence analysis and computer aided drug designing process

UNIT I Introduction to cheminformatics 15 HRS

Introduction-Branches of Cheminformatics- Genomics-Transcriptomics-proteomics-systems biology-functional genomics-metabolomics-structural genomics-Nutritional genomics- cheminformatics-molecular phylogency.Aims of Bioinformatics-Data acquisition-tools and Database development-data analysis-Data integration, Scope/Research areas of Bioinformatics- genome and sequence analysis from sequence to 3D structural prediction-analysis of genomewide biomedical data and functional genomics-database building and management-Training activities on Bioinformatics-research and development

UNITII Representation and Manipulation of 3D Molecular structure 15HRS

Introduction**,** experimental 3D data bases 3D pharmacophores, Implementation of 3D database searching, Theoretical 3D data bases-Structure-generation programs-conformational search and analysis- systematic conformational search-random conformational -other approaches to conformational search –comparison and evaluation of conformational search methods. Methods to derive 3DPharmacophorespharmacophoremappingusing constrained systematic search- clique detection-maximum likelihood method for pharmacophore Mapping- genetic Algorithm-other approaches to pharmacophore mapping - practical aspects of pharmacophore mapping, Applications of 3D pharmacophore mapping and 3D database searching

UNIT-III Similarity Methods 15 HRS

Introduction- similarity based on 2D finger prints, similarity coefficients-properties of similarity and distance coefficients –other 2D descriptor methods –maximum common sub graph similarity –reduced graph similarity, 3D similarity-alignment –independent methods –alignment methods –field based alignment methods-genomic projection methods –finding the optimal alignment comparison and Evaluation of similarity methods.

UNIT-IVData bases in Cheminformatics 15 HRS

Introduction-biological databases –history of biological databases-features of biological databases-classification scheme of biological databases-biological database retrieval systems.

Introduction-tools and databases of -NCBI –Database retrieval tool-Sequence submission to NCBI-Bankit-Sequin-BLAST-PSI-BLAST, RPS-BLAST-BLAST-BLAST 2 sequence

UNIT-VCheminformatics in computer- aided Drug design:

Introduction, drug discovery process- historical perspective-hit identification –structural bioinformatics in drug discovery –some basics about in silico drug designing-SAR and QSAR technique in drug design-development of linear –free energy relationships-application of Hammett equation-Hansch equation –application of QSAR in CADD. Molecular Docking-Introduction-flexibility calculation- Simulation techniques widely used in molecular docking-M D simulation - software for structure based drug design and molecular docking-A briefing on drug bank- auto dock-steps for flexible docking in auto dock –preparing the ligand and the macromolecule for auto dock-auto grid- auto dock file formats-choose the docking algorithm-viewing conformational clusters by RMSD

REFERENCES

1. Bioinformatics –Principles and Applications by Zhumurghosh&Bibekan and Mallick, Oxford university press I edition (2008)

2. An Introduction to Cheminformatics by Andrew R.Leach&ValerieJ.gillet- Springer International Edition, I Edition (2009)

INORGANIC CHEMISTRY PRACTICAL – III

(Subject code: 21PGCHP31)

Semester: III	Practical:7	Hours/W: 2	Credit: 1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1:recall the principle, theory and applications of gravimetric analysis (K2)

CO2: interpret the separation of ions in the mixture (K2)

CO 3:Assess the separation of binary mixture for various inorganic compounds by gravimetric method.

QUANTITATIVE ANALYSIS

Separation and estimation of the following mixtures by gravimetric and volumetric methods.

1. Nickel (G) and Copper (V)
2. Calcium (G) and Copper (V)
3. Barium (G) and Calcium (V)
4. Nickel (G) and Iron (V)
5. Zinc (G) and Copper (V)
6. Copper (G) and Calcium (V)

Note:

Students should submit their record note for evaluation at the time of examination.

Viva – Voce examination on practical will be conducted.

REFERENCES:

1) J.Mendhem, R.C. Denney, D. Barnes, M.J.K.Thomas, Vogel's Text Book of Quantitative Chemical Analysis, 6th edition, 2002, Pearson education Ltd.

2) V. Venkateswaran, R. Veeraswamy, A. R. Kulandaivelu, Basic principles of Practical Chemistry, 2nd edition, 1997, Sultan Chand &sons,Educational Publishers, New Delhi

INORGANIC CHEMISTRY PRACTICAL – IV
(Subject code: 21PGCH32)

Semester: III	Practical: 8	Hours/W: 2	Credit: 1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1: restate the principles of synthetic methodologies (K2)

CO3: demonstrate the synthesis of various Inorganic coordination complexes (K3)

CO4: categorize the complex preparation based on the conditions (K4)

PREPARATION OF INORGANICCOORDINATIONCOMPOUNDS

1. Tetramminecopper (II)sulphate
2. Tristhioureacopper(I)sulphate
3. Hexathiourea lead(II)nitrate
4. Potassiumtrioxalatochromate (III)
5. Hexaaquochromium(III)chloride
6. Hexamminecobalt(III)chloride
7. Sodiumhexanitrocobaltate (III)
8. Diaquobis(ethylenediamine)copper(II)iodide
9. Hexamminenickel(II)chloride
10. Tetramminenickel(II) chloride

Note:

Students should submit their record note for evaluation at the time of examination.

Viva – Voce examination on practical will be conducted.

REFERENCES:

1. R. Gopalan, V. Ramalingam, Concise Coordination Chemistry, 2001,VikasPublishingHouse Pvt. Ltd.
2. V. Venkateswaran, R. Veeraswamy, A. R. Kulandaivelu, Basic principles of Practical Chemistry, 2nd edition, 1997, Sultan Chand &sons,Educational Publishers, New Delhi

CORE – PRACTICAL ORGANIC CHEMISTRY – III
(Subject code: 21PGCHP33)

Semester: III	Practical:9	Hours/W: 2	Credit: 1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: recall the principle underlying estimation of organic compounds (K2)

CO2: establish the reactions of estimated organic compounds (K3)

CO3: estimate the organic compounds in the research laboratories and industry (K4)

CO4: adopt green synthetic methods to protect the environment(K5)

1. QUANTITATIVE ANALYSIS OF ORGANIC COMPOUNDS

(i) Saponification value of an oil

(ii) Iodine value of an oil

(i) Estimation of phenol

(iv) Estimation of glycine

(v) Estimation of methyl ketones

(vi) Estimation of glucose

(vii) Estimation of ascorbic acid

Note: Students should submit their record note for evaluation at the time of the examination.

Viva-Voce examination on practicals will be conducted.

REFERENCES:

1. Furniss, Hannaford, Smith, Tatchell.; *Vogel's Textbook Of Practical Organic Chemistry.*, Pearson Education.
2. Bhutani.S.P, ArunaChhikara.; *Practical Organic Chemistry*., Ane books India.
3. Gnanapragasam.N.S., Ramamurthy.G.; *Organic Chemistry Lab Manual*., S.ViswananathanPvt.Ltd.
4. Ahluwalia.V.K, Sunitha Dhingra, Adharsh Gulati.; *College Practical Chemistry.,* University Press.

CORE – PRACTICAL ORGANIC CHEMISTRY – IV
(Subject code: 21PGCH34)

Semester: III	Practical: 10	Hours/W: 2	Credit: 1

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: restate the principle underlying synthesis of organic analysis (K2)

CO2: design two stage preparations of organic compounds (K3)

CO3: establish the structure of synthesized organic compounds using spectral data(K3)

CO4: adopt green synthetic methods through the sophisticated instruments like microwave ovenandsonicator to protect the environment(K5)

CO 5: Design the new separation techniques in future (K6)

1. PREPARATION OF ORGANIC COMPOUNDS (DOUBLE STAGE)

(i) Aminoazobenzene from aniline

(ii) p-Nitroso-N,N-dimethyl aniline from N,N-dimethylaniline

(iii) Benzilic acid from benzoin

(iv) Acetylsalicylic acid from methylsalicylate

(v) Anthraquinone from phthalic anhydride

2. DEMONSTRATIVE EXPERIMENTS

(i) Experiments using TLC, Column and Paper chromatography

Note: Students should submit their record note for evaluation at the time of the examination.

Viva-Voce examination on practicals will be conducted.

REFERENCES:

1. Furniss, Hannaford, Smith, Tatchell.; *Vogel's Textbook Of Practical Organic Chemistry.*, Pearson Education.
2. Gnanapragasam.N.S., Ramamurthy.G.; *Organic Chemistry Lab Manual*., S.Viswananathan Pvt.Ltd.

SELECTED TOPICS IN CHEMISTRY

(Subject code: 21PGCH41)

Semester: IV	Core:10	Hours/W: 5	Credits: 5

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1: describe the principles of PES.(K2)

CO2:demonstrate the topochemical controlled organic solid-state reactions (K3)

CO3: examine the activity of enzymes action in biological system (K3)

CO4:analyze the chemistry of nanophase materials (K4)

CO 5: Justify the use of PES on Inorganic compounds (K5)

CO 6: Justify the applications of homocyclic and different dimensional molecules in Inorganic system (K5).

Unit- I: Organic Solid state chemistry 15hrs

Topochemical control of solid state organic reactions, Intramoleclar reactions - Conformational effects, Intermolecular reactions, Molecular packing effects, Photodimerization of orthoethoxy trans cinnamicacid(α, β, γ forms), Photo polymerization of 2,5-distyrylpyrazine, Photopolymerisation of diacetylenes, Asymmetric synthesis, dimerisation of Anthracene- role of crystal defects, Control of molecular packing arrangements, organic reactions with Inorganic host structures, Electrically conduction organic solids: Organic metals, conjugated system doped polyacetylene, poly para-phenylene, polypyrroleOrganic charge transfer complexes- New super conductors

Self-study: stereochemistry of organic solid-state compounds

UNIT-II Physical techniques in Inorganic Chemistry 15 Hrs

Photo electron spectroscopy (XPES and UVPES) – Basic principles - Istrumentation–sources of PES-photoelectric effect, ionization process-excitation and ejection of electrons-Vibrational structure-origin of fine structure - Koopman's theorem –photo electon spectra of N_2, O_2, H_2O, NH_3, CO, HCl, CH_4– Electron Spectroscopy for Chemical Analysis (ESCA)-chemical information from ESCA – Chemical shift- Applications of ESCA of the following compounds - N_2, NaN_3, CCl_3CH_3, $CF_3CO_2CH_2CH_3$, $[Co(en)_2(NO_2)_2]NO_3$, $PhSCH_2COOH$, bonding mode in $[M(N_2)L_4]$ complex-Using ESCA, distinguish between cysteine and oxidized cysteine, chlorocyclo phosphazine and Dimethylamino substituted phosphazine-Shake up and Shake off process –Auger electron spectroscopy (AES)- Auger effect.

Self-Study: X-ray Absorption analysis-EXAFS

Unit-III: Nanomaterials, Nanostructures and Properties 15 hrs

Basic Concepts- Graphene, Quantum wells, Synthesis techniques-top down, bottom up method-sol gel methodSolution based synthesis of Nanoparticles,Gold nanoparticles, Semiconductor and Oxide nanoparticles, Vapour-phase synthesis of nanoparticles via Solutions or solids, Template synthesis of nanomaterials using framework, supports and substrates, Characterisation and formation of nanomaterials,One dimensional control: carbon nanotubes and Inorganic nanowires, Two dimensional control: Graphene, Quantum wells,

and solid-state superlattices, Three dimensional control: Mesoporous materials,inorganic-organic nanocomposites

Self-Study: optical properties of Nanomaterials.

Unit- IV: Enzyme Chemistry 15hrs

Enzymes Metal biosite structures in enzymes, entatic state and enzyme action, Inhibition and poisoning, Metalloenzymes, Zinc enzymes – Carboxy peptidase and Carbonic anhydrase, Iron enzymes – Cytochrome C oxidase,Catalase, Peroxidase and Cytochrome P_{450}, Copper enzymes – SOD, Molybdenum oxatransferase enzymes, Xanthine oxidase

Self-study: Brief study on magnesium enzymes

Unit- V: Selected compounds in Inorganic chemistry 15hrs

Synthesis and Structure of compounds – chromium(II)acetate, manganese(III)acetate, manganese(III)oxalate, copper(II) acetate, solid nickel-DMG complex, zinc(II) acetate and zinc-EDTA complex, Prussian blue and Turnbull's blue, Zeolites- Natrolite, Sodalite, Boggsite and ZSM-5, Homocyclic Inorganic systems- S_8, S_4^{2+}, Se_4^{2+}, Te_4^{2+}, Squarate, croconate, rhodizonate, Cage compounds-P_4, P_4O_6, P_4O_7, P_4O_8, P_4O_9 and P_4O_{10}, Spinels and Inverse Spinels,Fullerenes, Carbon nanotubes and graphene

Self-study:Molecular materials and fullerides

REFERENCES

1. James E. Huheey, Inorganic Chemistry, Principles of structure and reactivity, 4th edition, Pearson Education
2. F.A.Cotton and G.Wilkinson – Advanced Inorganic Chemistry, 3rd edition, Pearson education.
3. Shriever& Atkins, Inorganic Chemistry, 5thedition., Oxford university press
4. E.A.V Ebsworth David W.H.Rankin Stephan Cradock, (1987), Structural Methods in Inorganic Chemistry, English Language Book Society/Blackwell Scientific Publications
5. Lippard, Berg, Bertini and Valentine, Bio-Inorganic chemistry,University Science Books
6. AsimK.Das, Bioinorganic chemistry, Books and Allied (p) Ltd.

EMERGING TRENDS IN PHYSICAL CHEMISTRY (THEORY)

(Subject code: 21PGCH42)

Semester: IV	Core:11	Hours/W: 5	Credits: 5

COURSE OUTCOMES:

As the course concludes the student will acquire the knowledge and able to

CO1: acquire in-depth knowledge on characteristics and structural arrangements of polymers (K3)

CO2: familiarize with the current and emerging research trends in biophysical, nano science. (K2)

CO3: remember the various characterization techniques available for of nano particle (K1)

CO4: analyze the structure and classification of proteins using modern spectroscopic techniques (K2)

CO5: gain knowledge about approximation methods, Born-Oppenheimer approximation and its application to one and two electron systems (K2)

CO6: understand and explore the quantum mechanical background of Molecular Orbital theory, Valence Band theory and hybridization (K3)

Unit I Polymers 15 Hrs

Overview and Classification of Polymers-Kinetics of polymerization - Free radical polymerization, Ionic – coordination – condensation polymerizations. Molecular weight of polymers and its determination, molecular weight by light scattering method and viscosity method.Vulcanization of rubber-Models of viscoelastic behavior, Hooke model – Newton model – Burger Maxwell model – Kelvin – Voigt model, Structure of crystalline, semicrystalline and amorphous polymers, Glass transition temperature (Tg) –factors influencing it. Elastomers – thermoplastic elastomers. Mechanical properties – deformation elastomers (thermodynamics, statistical theory)Plasticisation theory

Self-study: Conducting Polymers

Unit II Biophysical Chemistry 15 Hrs

Introduction - Levels of structure in biological molecules (primary, secondary, tertiary and quaternary) Forces that determine protein structure – hydrogen bonding, hydrophobic interaction, ionic interactions and disulfide bonds. Techniques for the study of biological structure, Spectroscopic analysis of biopolymers – far and near uv absorptions – effect of prosthetic groups,Fluorescence spectroscopy – basic principles – factors affecting intensity – experimental measurements – properties of typical fluorescent groups – Forster's theory of singlet – singlet energy transfer(*study of relevant parameters only*).

Electron microscopy – measuring electron diffraction of a solid – determining molecular structure.Neutron scattering – comparison with x-ray scattering – locating hydrogens – solvent contrast in neutron and x -ray scattering.

Self-study:Role of surfaces in amyloid formation & Analytical and digital techniques for the detection of the SARS-COV-2

Unit III Characterization and properties of NanoMaterials 15 Hrs

Introduction- characterization of nanomaterials – SEM & TEM – AFM-XRD-RAMAN. Properties of nanomaterials – atom like behavior – Physicochemical properties– Optical properties – Electrical and electronic properties – Mechanic properties – Magnetic properties – Redox properties – catalytic activity, Nanomaterials in medicinal field – diagnosis – biosensors – biolabelling – nano materials as therapeutic agents – drug delivery – dendrimers – gene therapy, Nano materials in energy production – photovoltaics – advances in hydrogen fuel cells – Thermoelectrics – piezo electrics – nano materials in rechargeable batteries and super capacitors.

Self-study:Quantum tunneling

Unit IV Advanced quantum chemistry – I 15 Hrs

Approximation methods – Need for approximation, Perturbation theory – Time independent Perturbation (First order only), Application of perturbation theory to particle in one dimensional box, anharmonic oscillator and helium atom.Principle of variation method and its proofVariation methods and its applications to hydrogen atom and heliumatom.

Self-study:Symmeric and anti-symmetric wave functions & Pauli's exclusion principle

Unit V Advanced quantum chemistry – II 15 Hrs

The Born – Oppenheimer approximation, MO & VB theories as applied to hydrogen molecular ion (H_2^+) and hydrogen molecule, Coulomb integral exchange integral and overlap integral, Construction of sp, $sp^2$and sp^3 hybrid orbitals, Huckel molecular orbital theory – principles and applications to ethylene, butadiene and benzene, Huckel calculation of pi-electron energies.

Self-study: Pi electrons energy calculationof Napthalene &Electron spin and spin orbitals

REFERENCES:

UNIT I

1. R.J. Young and P.A. Lovell 'Introduction to Polymers', First Indian reprint, 2004, Viva
2. Gowarikar V.R et al., Polymer Science, 1986, Wiley Eastern Ltd,

UNIT II

1. Charles R. Cantor and Paul R. Chimnael, 'Biophysical chemistry' Parts I, II and III, W. H. Freeman and Company
2. AvinashUpadhyay,Kakoli Upadhyay and Nirmalendu Nath, Biophysical chemistry, Himalaya Publishing House

UNIT III

1. T.Pradeep, "Nano: The essential", 2007, Mc-Graw-Hill education.
2. B.Viswanathan, Nano materials, Narosa publications
3. S.Shanmugam, Nanotechnology, MJP publishers

UNITS IV & V

1. A.K. Chandra – Introductory quantum chemistry, 4^{th} ed (2001 reprint) Tata Mc Graw-Hill.
2. Donald A McQuarrie – Quantum Chemistry, Indian edition , Viva Books Pvt, Ltd.
3. Ira N.Levine – Quantum chemistry, 4^{th} ed, 1991, Prentice Hall of India.
4. Peter Atkins, Julio de Paula – Atkins' physical chemistry, 7^{th} ed, 2002, Oxford University Press

COMPREHENSIVE CHEMISTRY

CODE: 21PGCHS41

Semester: IV	CORE: 12	Hours/W: 0	CREDIT – 2

THIS PAPER IS PURELY INTERNAL AND THE STUDENTS HAVE TO STUDY ALL THE SUBJECT THEY HAVE LEARNT IN THE PREVIOUS SEMESTERS. OBJECTIVE TYPE ONLINE EXAMINATION WILL BE CONDUCTED. IT IS A SELF STUDY PAPER.

ANALYTICAL AND GREEN CHEMISTRY

(Subject code: 21PGCHE41)

Semester: IV	Elective:4	Hours/W: 4	Credits: 2

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1: Explore separation of compounds using chromatographic techniques (K2)

CO 2: differentiate the Principles involved in thermo-analyticaland electro analytical techniques(K3)

CO 3: Assess the values of analytical techniques in various industries (K5)

CO 4: Categorize the applications of Analytical techniques in life situation(K4)

CO 5: restate the principles of green chemistry (K2)

CO 6: integrate the applications of microwave assisted reactions in novel synthesis (K6)

Unit I: Chromatographic Techniques **9 hrs**

Separation methods- principle, Instrumentation and applications Classification of Chromatographic techniques, Partition Chromatography, Liquid-liquid chromatography, Paper chromatography, Gas liquid chromatography, Adsorption chromatography, Column chromatography, Thin-layer chromatography, Ion-exchange chromatography, HPLC.

Self-study:Elementary concepts of UHPLC

Unit II: Thermoanalytical techniques **9 hrs**

Thermoanalytical techniques –principle, instrumentation and application-TGA- Principle, instrumentation and factors affecting thermogram-Decomposition of Calcium oxalate monohydrate and copper sulphate pentahydrate

DTA-Principle and instrumentation-Thermal behavior of copper sulphatepentahydrate by DTA

DSC- Principle and instrumentation-Determination of purity of pharmaceuticals-Phase transition studies by DSC-study of glass transition temperature

Self-study:Online analyzers

Unit- III: Electroanalytical Techniques **9hrs**

Electroanalytical technique- Principle,Instrumentation (Block diagram) and applications.Electrogravimetry,Electrolytic separation and estimation of metal ions-Coulometry-Controlled potential coulometry-Coulometric titrations-separation of Nickel and Cobalt. Voltammetry- Principle, Instrumentation (Block diagram) and Applications-Stripping Voltammetry -Chronopotentiometry

Self-study:Ampherometry – principles and applications

Unit- IV: Spectro Analytical methods **9hrs**

Spectro-analytical methods – principle and applications,Colorimetry,Spectrophotomerty, Fluorimetry, Phosphorimerty, Nephelometry, Turbidimetry,Atomic absorption spectroscopy and Atomic emission spectroscopy

Self-study:Colourimetric estimation of Potassium ferrocyanide

Unit-IV: Green Chemistry **9 hrs**

Green chemistry - Principles of green chemistry, Prevention of waste/by -products,Maximum incorporation of the reactants into the final product,Prevention (or) minimization of hazardous products, Designing safer chemicals,Energy requirements for synthesis, Selection of appropriate solvent,Selection of starting material,Use of protecting groups and catalyst, Products designed should be biodegradable, designing of manufacturing plants, strengthening of analytical techniques.

Microwave induced green synthesis - Introduction and Applications. Microwave assisted reactions in water: Hofmann elimination, hydrolysis and oxidation of toluene. Microwave solvent free reactions: Deacetylation, Deprotection, Saponification of ester and Synthesis of nitriles from aldehydes

Self-study: Microwave assisted organic reactions

REFERENCES

1. Douglas A. Skoog and Donald M.West, Principles of Instrumental Analysis, 3rdedition, Saunders College Publishing.
2. Willard,H. H., MerritL.L.,Dean J.A., Instrumental Methods of Analysis, 7thedition,2008, CBS publishers, New Delhi.
3. J.Mendhem, R.C. Denney, D. Barnes, M.J.K.Thomas, Vogel's Text Book of Quantitative Chemical Analysis, 6th edition, 2002, Pearson education Ltd.
4. Skoog, D. A., West D. M., Holler, J.F., Fundamentals of Analytical chemistry,8th edition, 2006, Thomson Asia Pvt. Ltd., Singapore.
5. Paul T. Anastas,John C Warner, Green Chemistry, Theory and practice, 1998, Oxford University press, New York
6. V. K. Ahluwalia, Green Chemistry: A Text book, 1st edition, 2013, Narosa publishing house, New Delhi.

BIOCHEMISTRY

(Subject code: 21PGCHE41)

Semester: IV	Elective:4	Hours/W: 4	Credits: 2

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO1: summarize the nomenclature, structure and properties of amino acids, proteins, enzymes,lipids and vitamins (K2)

CO 2: classify biomolecules and discuss their reactions(K4)

CO 3: illustrate the biological role and importance of metabolites (K3)

CO 4: interpret the mechanistic pathway of the metabolic process (K4)

CO 5: assess the various deficiency diseases and the ways to prevent them to lead a healthy life (K5)

Unit I: Amino acids, Proteins **9 HRS**

a) Amino acids-General structure of amino acids- physical and electrochemical properties. Peptides - peptide bond- representation of peptide chain-naming of peptide chain-determination of the amino acid sequence of a polypeptide-biological role.

b) Proteins-Importance – classification based on shape of protein molecule and biological function- denaturation and renaturation –structure of proteins- color reactions of amino acids.

UNIT II Enzymes **9 HRS**

Introduction-importance-nomenclature and classification- biological role of enzymes-applications of enzyme - chemical nature – characteristics -mechanism of action of the enzyme chymotrypsin- Michaelis-Menten hypothesis- Lineweaver Burk equation - active site – mechanism of enzyme action -Fishers lock and key model, Koshlands induced fit model-modifiers of enzyme activity-inorganic modifiers-regulation of enzyme activity-organic modifiers-reversible enzyme inhibition- competitive, non- competitive and allosteric inhibition -Irreversible enzyme inhibition.

UNIT III Metabolism **9 HRS**

Definition and terminology of metabolism – functions of metabolism-glycolysis: general considerations,two phases, enzymes involved, kinds of reactions, reaction steps and stoichimetry of glycolysis. Citric acid cycle: enzymes involved, overview, reactions, stoichiometry, energy yield and role of water in the citric acid cycle, urea cycle.

UNIT IV Lipids **9 HRS**

Definition-classification based on chemical composition, simple lipids: fats and oils-difference between animal and plant fats-waxes-compound lipids: phospholipids, glycolipids and gangliosides-derived lipids. Physical properties and chemical properties - saponification, hydrolytic and oxidative rancidity, hydrogenation and acrolein test – quantitative tests-importance and biological role of lipids.

UNIT V Vitamins **9 HRS**

a)Definition-General characteristics- Classification- Storage of Vitamins in the body-Daily human requirements of Vitamins- Avitaminoses.

b)Fat soluble Vitamins: Vitamin A- Vitamin D- Vitamin E-Vitamin K- Coenzyme Q-Stigmasterol.Water soluble Vitamins:Vitamin B complex-Vitamin $B_{1,}$Vitamin $B_{2,}$Vitamin $B_{3,}$Vitamin $B_{5,}$ Vitamin $B_{6,}$Vitamin $B_{7,-}$ Vitamin $B_{9,}$Vitamin B_{12} ,Vitamin C.

Reference Books:

1. J.L. Jain (1983), "Fundamentals of Biochemistry", S. Chand &company Ltd. IV edition.
2. U. Satyanarayana,U Chakrapani Fundamentals of Bio Chemistry, 2008, Books and allied private ltd.,

CORE – PHYSICAL CHEMISTRY PRACTICAL – III
(Subject code: 21PGCHP41)

Semester: IV	Practical:11	Hours/W : 4	Credit : 2

By the end of the course, the students will be able to

CO1: Are able to communicate the results of their work to chemists and non-chemists

CO2:Use different instrumental methods of analysis and estimation

CO3:Optimize the reaction conditions for the intended product.

CO4:Analyse and interpret the data.

1. Comparison of acid strengths by studying the kinetics of acid catalyzed iodination of acetone.
2. Determination of rate constant of the redox reaction between potassium iodide and persulphate and verification of Bronsted Bjerrum equation.
3. Determination of thermodynamic parameters of an acid catalyzed hydrolysis of an ester.
4. Determination of partition coefficient for the distribution of iodine between CCl_4 and H_2O and the equilibrium constant of the equilibrium $KI + I_2$------ KI_3
5. Verification of Huckel-Bronsted equation of benzoic acid as weak electrolyte and to determine the concentration of a given solution of chloride using Huckel-Bronsted equation.

REFERENCES

1 Dr.K.Karunakaran, Laboratory manual in physical chemistry.

2. V.D. Athawale and Parul Mathur, Experimental physical chemistry, 2001 New age international publishers.

3. Lab manual supplied by the department

NOTE

Students should submit their record note for evaluation at the time of examination. Viva voce examination on practicals will be conducted

EXTTRA CREDIT COURSES (ECC)

INDUSTRIAL CHEMISTRY

(Subject code: 21PGCHEC11)

Semester: I	**Credits: 2**

COURSE OUTCOMES:

By the end of the Course the student will be able to

CO 1. Understand the ethical, historic, philosophical, and environmental dimensions of problems and issues facing industrial chemists.(K2)

CO 2.Know about fuels, composition, carbonization of coal, gasification, liquefaction, and coal tar based chemicals and layout for key processes in oil refining. (K1)

CO 3. Summarizes the raw materials and manufacturing of glass and cement industry(K3)

CO 4. Gain sound knowledge of inorganic materials like silicates, ceramics and cement (K1)

CO 5. Conclude the role of petroleum and petrochemical industry, composition, applications, process-cracking. Increasing demand of non-petroleum fuels, synthetic fuels. Petrochemical.(K5)

CO 6. Develop skills to estimate various components of fertilizers (K6)

UNIT I Cement and Ceramics

Cement -Composition-Types. Portland cement - Composition- Types - Manufacture (Wet and Dry process)-Uses,Setting of cement,Ceramics, Composition- Classification-Manufacture-Properties-uses

UNIT II Glass and Matches

Glass- Composition-Types-Formation operations -Melting-Blowing-Pressing-Annealing and finishing-Matches -Composition-Types-Manufacture - Safety matches

Unit III Pigments, Dyes and Paints

Pigments-Classification-Manufacture-Uses,Dyes-Classification-Preparation-Dyeing processes,Paints- Composition-Types-Manufacture-Testing of Paints

Unit IV Plastics and Fibres

Fibres- Natural- Synthetic fibres-Artificial silk-Rayon-Nylon-Trylene.Plastics-Composition-Classification-Manufacture-Properties -Uses

Unit V Fertilizers and Fuels

Fertilizers- Organic fertilizers- Inorganic fertilizers -Preparation –UsesFuels-Energy resources

Industrial gases-Water gas- Producer gas-Oil gas, Natural gas-Coal gas-Gobar gas-Indane gas-Petroleum products and coal products.

REFERENCES:

1. B.K. Sharma, Industrial Chemistry, Goel Publishing house Meerut.
2. R.K. Das, Industrial Chemistry.
3. C.N. Sawyer, P.L. McCarty and G.S. Parkin, Chemistry for environmental engineering and science.
4. F. W. Bilmayer, Text Book of Polymer Science, John Wiley & Sons, 1994.
5. A. Rudin, The Elements of Polymer Science and Engineering.
6. P. Ghosh, Polymer Science and Technology of Plastics and Rubbers.

ENVIRONMENTAL CHEMISTRY

(Subject code: 21PGCHEC21)

Semester: II	**Credits: 2**

COURSE OUTCOMES:

By the end of the course the student will be able to

CO 1. Describe the effect of toxic elements on environmental and biological systems.
CO 2.Demonstrate knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil. K3
CO 3. Recognize different types of toxic substances & responses and analyze toxicological information.
CO 4. Translate the basic chemical concepts to analyze chemical processes involved in different environmental problems (air, water & soil).
CO 5. Describe experimental methods for analysis of water and soil analysis and pollution awareness to society.
CO 6. Describe the air, water, pollution by diffract industry, pesticides, microorganism.

UNIT I Environmental Chemistry:

Concept and scope of Environmental Chemistry-Acid base reactions -pH and pOH- Ionic product of water- Common ion effect - Buffer solutions-Solubility and solubility product-Oxidation and reduction -Chemistry of Environmental Trace Elements: Pb, As, Hg and Cd

UNIT II Atmospheric Chemistry:

Chemical composition of the atmosphere,Chemical and photochemical reactions in the atmosphere, Formation of smog,PAN,Acidrain,Oxygen and ozone chemistry, Catalytic decomposition process of ozone Concept of atmospheric aerosol Chemistry,Green house gases

UNIT III Water Chemistry:

Physical and chemical properties of terrestrial,Marine water and their environmental significance,Water quality parameters- Physical, chemical and biological,Distribution of chemical species in water; Gases, organic matter and humus matter in water.

UNIT IV Soil Chemistry:

Chemical & mineralogical composition of soil,Physical properties of soil,Texture-Bulk density-Permeability, Chemical properties -Cation exchange capacity-pH,Macro and micro nutrients

UNIT V Chemistry of Organic compounds:

Soap,Detergents, Bleaching agents,Chemistry of colloids,Hydrocarbons- PAH-PCBs,Phenols,Chlorofluorocarbons, Pesticides,hemical fertilizers

REFERENCES:

1. A. K. De, Environmental Chemistry.
2. B.K. Sharma, and H. Kaur, Environmental Chemistry.
3. S. E. Manahan, Environmental Chemistry.
4. J. W. Moore and E. A. Moore, Environmental Chemistry.
5. G. W. Vantoon& S. J. Duffy, Environmental Chemistry - A global perspective, Oxford university Press
6. H. Koren, Handbook of Environmental Health and Safety – Principle and practices, Vol. II, Lewis Publishers

HEALTH CHEMISTRY

(Subject code: 21PGCHEC31)

Semester:III	**Credits: 2**

COURSE OUTCOMES:

By the end of the course the student will be able to

CO 1. Understanding of the basic biological and pharmacological interactions by using both natural products and total synthesis of bioactive molecules.
CO 2. Demonstrate basic first aid skills needed to control bleeding, ill or injured person and immobilize injuries.
CO 3. Demonstrate skills to provide one- and two- person cardiopulmonary resuscitation to infants, children and adults.
CO 4. Recognize the different types of blood lipid, discuss the metabolism of fatty acids and analyze the factors influencing the absorption of cholesterol.
CO 5. Compare the digestion and absorption of carbohydrates, processes involved in their metabolism and regulation of blood sugar.
CO 6. Identify the function and properties of blood, bile pigments and bile acids

UNIT I Health

Definition: Food, Food Pyramid - Health-Hygiene- mal-, under- and overnutrition, their causes and remedies, sanitation, Carbohydrates -Protein- Classification and its Biological functions

Vitamins – Classification and its Biological functions.

UNIT II Drugs

Drugs- Types of drugs,Depressant,Anticonvulsant,Narcotics,Antipyretics, Antibiotics, Antiseptics, Analgesics,MuscleRelaxants,Cardiovascular,Vasodepressants, Steroids

Unit III Body fluids

Blood Volume, Blood groups,Coagulation,Blood Pressure, Anemia, Blood Sugar, Hemoglobin- Chemistry Of Respiration-Urine-Electrolyte Balance.

Unit IV Enzymes, Hormones, Digestion

Types of enzymes, Enzyme Action,Characters of Hormones- Action,Examples of Essential Hormones-DigestionoIn Mouth- Stomach-Intestine- Pancreas,Mineral Metabolism

Unit V First Aid for Accidents and Indian Medicinal Plants and Trees

Rules of first aid,Cuts, Abrasions and bruises, Bleeding, Fractures, Burns, Fainting, Poisonous bites,First aid box,Antidotes for poisoning, Uses of Plant extracts for medicinal

purposes - AdathodaVasica, Hibiscus Rosa –Sinensis, Cynodondactylon, Tinospora cordifolia

REFERENCES

1. Deb A C, Fundamentals of Biochemistry, New Central Book Agency, Calcutta, (1994).
2. Satake M and Mido Y, Chemistry for Health Science, Discovery Publishing House, New Delhi, (2003).
3. Jayashree Ghosh, A Text book of Pharmaceutical Chemistry, S. Chand and Co.Ltd, (1999).
4. Ashutosh Kar, Medicinal Chemistry, Wiley Easterns Limited, New Delhi, (1993).
5. Alex V Ramani, Food Chemistry, MJP Publishers, Chennai, (2009).

ANALYTICAL CHEMISTRY

(Subject code: 21PGCHEC41)

Semester:IV	**Credits: 2**

COURSE OUTCOMES:

By the end of the course the student will be able to

CO 1 Understand the various types of precipitation and analyze the theories of precipitation.

CO 2.To describe the basic concept of analytical chemistry. Qualitative and quantitative analysis.

CO 3. Describe the different separation techniques such as distillation, Solvent and Solid Phase extraction.

CO 4. Be familiar with calculations in analytical chemistry, be able to calculate titration errors for method evaluation, and perform statistical evaluation of results from classical and instrumental chemical experiments and analyses

CO 5. - Make scientific reports from chemical experiments and present the results in a transparent manner

CO 6. Understanding the knowledge of intellectual property rights

UNIT I Basic Concepts in analytical techniques

SI Units, Definitions of the Seven Base Units (Mass, Length, Time, Temperature, Amount of substance, Electrical current and Luminous intensity),Derived units, Conversion between units,Significant figures.

Unit II Chemical Concentrations

Mole, molar mass,Calculations in grams and moles, Solutions and their concentrations:

Molar concentration- Percent concentration -Parts per million/billion (ppm, ppb)- Volume ratios for dilution procedures. Preparing solutions-standard solutions- primary standards, secondary standards-Preparation of buffers.

Unit III Solvent Extraction

Distribution law,Determination of distribution ratio Batch extraction,continuous extraction, discontinuous extraction,counter current extraction

Unit IV Gravimetric Analysis

Properties of precipitates and precipitating reagents,Particle size-Filterability of Precipitates (factors that determine particle size, formation of precipitates and particle size),Colloidal Precipitates (coagulation of colloids, peptization of colloids, treatment of colloidal precipitates),Crystalline Precipitates (particle size and filterability),Co-precipitation (surface adsorption, mixed-crystal formation, occlusion, and mechanical entrapment, co precipitation errors),Precipitation from Homogeneous Solution (The use of the technique of homogeneous solutions to effect precipitation),Drying and Ignition of precipitates

Unit V Introduction to Intellectual Property

Introduction, Different Types of IP- Copyrights-Trade Marks-Patents-Industrial Designs-Trade Secrets, Importance of protecting IP

References:

1. Douglas A. Skoog and Donald M.West: Fundamentals of Analytical Chemistry
2. N.K. Acharya: Textbook on intellectual property rights, Asia Law House (2001).

Allied Chemistry-I (for Bot and Zoo)
(Subject code:21UCHA11)

Semester: I	Allied: A1	Credits : 4	Hours/W :4

Objectives:

- To know the structure and properties of compounds
- To understand the concepts of redox system and types of reactions
- To identify the intermolecular forces in different molecules.
- To Study the chemistry of carbon and nitrogen compounds
- To Know the synthesis of important aminoacids.

Outcome: Students Can

- Identify bonding and structure of organic and inorganic compounds
- Familiour with the acid-base conceps and their applications
- Understand the role of hydrogen bonding and other molecular forces through different applications
- Get the knowledge of different functionalities and their properties
- Assimilate the importance of protiens and aminoacids in biological systems.

Unit I: Chemical Bonding **12 hrs**

Valency and valence electrons - Electronic theory of valency -Electrovalecy-conditions favouring electrovalency-illustration -Electrovalent compounds and their properties - covalency- conditions favouring covalency-illustration- Covalent compounds and their properties-Coordinate covalency-conditions favouring formation of the bond-illustration- Transition from electrovalency to covalency- polarisation and polarizability-Fajan's rules-statement and illustration- Atomic orbitals-Definition-charge cloud interpretation-shapes of s,p and d orbitals- Overlappin gof atomic orbitals-conditions for overlap-types(s-s, s-p,and p-p) with illustrations-sigma and pi overlaps- hybridisation sp^3 in CH_4, sp^2 in BF_3 and sp in $BeCl_2$. Geometry of H_2O and NH_3 molecules-VSEPR theory.

Self Study: Atomic number, mass number, isotopes, electronic configuration of atoms and ions.

Unit II: Redox systems and analytical chemistry-I **12 hrs**

Redox systems- Redox reactions in terms of electron transfer - Oxidation number-Definition-Rules for assigning oxidation number- Calculation of oxidation number- Redox processes in terms of oxidation number- Advantages and disadvantages of the concept- Acids and bases-Arrhenius concept –illustration- Lowry-Bronsted concept-conjugate acid and conjugate base - Types of reactions relevant to qualitative analysis - Displacement reaction – Decomposition - Double decomposition- Hydrolysis- redox reaction- Complex formation- Interfering anions and their elimination- Group reagents and analytical group classification- Explanation and application of the following principles in qualitatiive analysis- Solubility and solubility product- Common ion effect- pH- Buffer

Self Study: oxidation, reduction, acids and bases.

UNIT III: Intermolecular forces and properties of liquids 12 hrs

Polar and non-polar molecules - Dipole-dipole (Debye) forces, dipole-induced dipole (Keesom) forces, Induced dipole-Induced dipole (London) forces. Repulsive forces - Resultant intermolecular energies- Hydrogen bonding-Nature of hydrogen bonding-conditions favouring hydrogen bonding- Types of hydrogen bonding-illustrations-impact of hydrogen bonding on melting points, boiling points and solubilities. Electrolysis - What is electrolysis-strong and weal electrolytes - Mechanism of electrolysis - Electrical units-coulomb,Amphere, Ohm and Volt- Faradays laws of electrolysis and their importance - Conductance of electrolyte – Conductance- Specific conductance and molar conductance-Units - of equivalent conductance with concentrations

Self Study: pure covalent bonds with examples, electro negativity, conductors, insulators, boiling point, melting point

UNIT IV: Aldehydes, Ketones, Acids and Amides 12 hrs

Aliphatic aldehydes and ketones-Nomenclature-General reactions- Formaldehyde- a comparison with other aldehydes of the series - Aromatic aldehydes-Reactions of benzaldehyde-benzaldehyde compared with acetaldehyde - Aromatic ketones-Aceton, acetophenone and benzophenone-distiction- Aliphatic saturated monocarboxylic acids-Nomenclature, general reactions-comparison of formic acid with other acids of the series. Aromatic saturated monocarboxylic acids-distinction between benzoic acid and acetic acid - Aliphatic amides-nomenclature, general reactions - Aromatic amides-Distiction between benzaldehyde and acetamide.

Self Study: aliphatic compounds, aromatic compounds, Functional group of aldehydes, ketones and amides

UNIT V: Amines, Amino acids and Proteins 12 hrs

Aliphatic monoamines - Nomenclature and classification - General reactions- Aniline-Reactions of aniline- Distinction between aniline and ethylamine- Amino acids-classification-zwitter ions-isoelectric point-preparation and properties of glycine and alanine- Proteins-introduction-peptides and polypeptides-partial hydrolysis and terminal residue analysis in the determination of structure of peptides.

Self Study: Functionalities of amino acids and amines, Functionalities of proteins (nitrogen containing compounds)

NOTE : Course materials will be supplied to the students**.**

Allied Chemistry Practical-I (For BOT and ZOO)
Inorganic qualitative analysis
(Subject code:21UCHAP11)

Semester : I	**Allied : AP1**	**Credit :1**	**Hours/w :2**

Qualitative anlysis of a simple salt containing one anion and one cation

Anions :Carbonate, Borate, Fluoride, Oxalate and Phosphate
Cations : Lead, Bismuth, Copper, Cadmium, Cobalt, Nickel, Manganese, Zinc, Barium, Strontium and Ammonium

Note: Laboratory manual will be supplied.

Allied Chemistry-II (for Bot and Zoo)
(Subject code:21UCHA21)

Semester: II	Allied: A2	Credits : 4	Hours/W :4

Objectives:

- **To understand and correctly use thermodynamic terminology.**
- To describe the composition and properties of colloidal dispersions and surface phenomena
- To distinguish between monosaccharides, disaccharides, and polysaccharides
- To study the special arrangement of atoms in a molecule and know how role of hetero atoms in organic compounds
- To understand the basic concepts of quantitative analysis

Outcome: Students Can

- **Explain fundamental thermodynamic properties**
- List and explain several technological applications of colloids
- Summarize the roles carbohydrates, alkaloids and terpenoids play in biological systems.
- Figure out how many stereoisomers a compound has, and synthesis of a few heterocyclic molecules.
- Prepare and standard solutions and standardize an unknown solution.

Unit-I : Thermodynamics **12 hrs**

Thermodynamic equilibrium - Process and types: Isothermal, adiabatic, isochoric, isobaric, cyclic, reversible, and irreversible- comparison between isothermal and adiabatic processes, reversible and irreversible processes - Internal energy as a state function- components of internal energy- Work: Thermodynamic concept-types of work - Heat : Thermodynamic concept- Heat and work as path functions - First law of thermodynamics- Statement of the law of conservation of energy- Mathematical expression of the law- Application of the law- Heat capacity, specific heat capacity and molar heat capacity of asystem- Relation between molar hear capacities of gases- Enthalpy and enthalpy change- Enthalpy as a state function- Relation between ΔH and ΔE- Enthalpies of reaction, formation and combustion-Definition and illustration- standard state- Calculation of enthalpy change using Hess law- Bond enthalpies and bond dissociation enthalpies-Definition and illustration using CH_4 as example (Numerical problems not expected)- Spontaneous (natural) process- Entropy-it's meaning of disorder- Gibb's free energy-its meaning as available energy- Criteria for spontaneity

Self study: ideal gas, ideal gas equation, homogeneous reactions and heterogeneous reactions, heat.

Introduction - Basic terminology and functional concepts- System, boundary and surrounding- Types of systems: open, closed and isolated- Properties of a system: extensive and intensive - State of a system and state variables (or state functions)

UNIT : II Surface chemistry and Colloidal Chemistry 12 hrs

Adsorption chemistry-introduction-definition-distinction from adsorption- Adsorption and adsorbate-definition and explanation- Chromatography-introduction- Adsorption chromatography-column chromatography, TLC- Partition chromatography-ascending chromatography- R_f value and its significance- Ion exchange chromatography-gas liquid chromatography (GLC), high - Types of colloidal systems- Classification of colloids-Lyophilic and lyophobic sols-a comparison- Stability of colloids-origin of charge-electrical double layer-salvation- Electrical properties-electrophoresis and electro-osmosis- Gels-gelation-classificatio-properties of gels-hydration, swelling or inhibition, syneresis and thixotropy- Emulsions-types of emulsion-identification of emulsion-dilution test, dye test, spreading test, viscosity and electrical conductivity-de-emulsification- Application of colloid in food, medicine, industry, purification of water, artificial rain, blue colour of the sky and cleaning action of soap.

Self study: Adsorbent, adsorbate, molecular interactions.

UNIT : III Carbohydrates, Alkaloids and Terpenoids 12 hrs

Introduction- Monosaccharide- Reaction of glucose- Open chain structure and ring structure of glucose (elucidation not expected)- Epimers, mutarotation- Interconversion of glucose into fructose and vice versa- Disaccharides- Reactions and structure of sucrose (elucidation nor expected)- Structure of maltose and lactose (elucidation not expcted)- Polysaccharide- Starch- amylase and amyl pectin-type of glycosidic linkage- Reaction of starch-action of heat-, hydrolysis and with iodine- Alkaloids- Definition, classification, (based on structure) occurrence and extraction- General methods of identification-functional nature of oxygen-functional nature of nitrogen-unsaturation-exhaustive methylation-Structure of conine- Terpenoids- Introduction, classification of terpenoids-Isoprene rule-Structure of citral (synthesis not included)

Self study: Examples for food contains carbohydrates

UNIT : IV Stereoisomerism and Heterocyclic compounds 12 hrs

Optical isomerism- Plane polarized light - Optical activity - Asymmetric carbon-chirality - Elements of symmetry-plane of symmetry- axis of symmetry-centre of symmetry-dissymmetric- Van't Hoff-le Bel theory- Optical isomerism of tartaric acid- Racemization - Resolution of racemic-mixture-biochemical method, chemical method and chromatographic method- Geometrical isomerism- Cause for geometrical isomerism- Illustration of compounds containing C-C double bond - Heterocyclic compounds- Pyrrole- Introduction-aromatic character- Basic and acidic character of pyrrole- Pyridine- Electronic interpretation of electron-rich centers- Reaction of pyridine- Quinoline- Skaraup synthesis - Reactions of quinoline

Self study: Isomers, cyclic compounds, practice to draw the structure of simple molecules like H_2O, NH_3

UNIT : V Analytical Chemistry-II 12 hrs

Methods of expressing concentration of solution- Normality- Molarity- Molality-Mole fraction- Equivalent weight of acids, bases, oxidizing agent and reducing agent-Standard solution- Primary standard- Secondary standard-Preparation of standard solution-

Principles underlying the following types of titration-Acid-base titration-theory of indicator-Permanganimetry-Dichrometry-Iodometry and Iodimetry-EDTA

Self study: Solvent, solute, solution, saturated solution, unsaturated solution, equivalent weight.

Note: Course materials will be supplied to the students.

Allied Chemsitry Practical-II (For Bot and Zoo)
Inorganic Volumetric Estimations
(Subject Code : 21UCHAP21)

Semester : II	Allied AP2	Credit : 1	Hours/W : 2

S.NO	Estimation	Link	Standard
1	Strong acid	Weak base/ Strong base	Strong acid
2	Strong acid	Strong base	Weak acid
3	Strong base	Strong acid	Weak base
4	Oxalic acid	Potassium permanganate	Oxalic acid
5	Ferrous sulphate	Potassium permanganate	Ferrous ammonium sulphate
6	Potassium dichromate	Ferrous sulphate	Potassium dichromate
7	Ferrous ammonium sulphate	Potassium dichromate	Ferrous sulphate
8	Potassium permanganate	Sodium thiosulphate	Potassium dichromate
9	Magnesium sulphate	EDTA	Zinc sulphate
10	Zinc sulphate	EDTA	Magnesium sulphate

Note: Laboratory manual is supplied.

ALLIED CHEMISTRY 1 (FOR PHYSICS)

SUBJECT CODE:21UCHA31

Semester: III	Core : 1	Credits : 4	Hours / W : 4

OUTCOMES:

- Understanding atomic structure and periodicity
- Appreciating the mistery of existence of atoms together in molecular form
- Enjoying the regularity in solids
- Understanding acids and bases and redox process
- Application of learnt knowledge in practicals.

UNIT 1 ATOMIC STRUCTURE AND PERIODIC TABLE 12 hrs

ATOMIC STRUCTURE

Bohr model of atom- Atomic spectrum of hydrogen and Bohr theory - Refinement of the Bohr theory- Duel nature of electrons particles or waves- Quantum numbers and its significance- Uncertainty principle- Paul's exclusion principle, Hund's rule- Periodic table- Modern periodic table- Long form of periodic table- Division of elements into s,p,d and f blocks-Bohr's aufbau principle electronic configuration of ground state of atoms up to K(Z=19)-Trends in atomic properties Ionization energy, successive ionization energy , electron affinity, electro negativity Pauling, Mulliken and Allred Rochow's scale

UNIT II STRUCTURAL AND CHEMICAL BONDING 12 hrs

Types of chemical bond - Electrovalent bond (conditions for formation and associated properties)- Covalent bond (conditions for formation and associated properties)- Coordinate covalent bond- Orbital overlap ss, sp, pp overlap- Sigma and pi bond formation of N_2 and O_2 properties- Polar and non-polar molecules- Dipole moment and its applications- VSPER theory application to CH_4 , NH_3 and H_2O - Molecular orbital theory, bonding, antibonding and non-bonding orbitals- MO diagrams for H_2 , He_2 and O_2 bond order

UNIT III SOLID STATE AND ENERGETICS 12 hrs

Macroscopic properties of solids- Types of characteristics of crystals- Covalent solids structure and properties of diamond and graphite- Ionic crystals solid NaCl- Metallic crystals- Molecular crystals intermolecular forces- Metals free electron theory and bond theory of metallic bond- Superconductors- Lattice energy- BornHaber cycle- Law of conversation of energy- Enthalpy of reactions- Entropy and Gibbs energy- Relationship between Gibbs energy and equilibrium-

UNIT IV ACID, BASES AND REDOX PROCESSES 12 hrs

Concept of acids and bases- Arrhenius concept- Bronsted Lowry concept conjugate acids and bases- Lewis concept- Effect of solvents and substituents on relative strengths of acids and bases- Hydrolysis- Ionization of water- pH scale definition of pOH , pK_a, pK_b simple numerical problem- Buffer solution - Redox processes- Electronic concept of oxidation and reduction- Oxidation number rules- Calculation of oxidation number of elements in neutral molecules and in ions- Balancing ionic equation by oxidation number method-

UNIT V PRACTICAL CHEMISTRY1 12 hrs

Introduction acquaintance with chemical laboratory laboratory equipments solid reagents, liquid reagents and test papers laboratory instructions and some don'ts Bunsen burner (self study) -Chemistry involved in the analysis of anion and cations - Dry tests (action of heat, flame test, filter ash test) -Wet test (with acids , with Na_2CO_3 extract)- Elimination of interfering anions and preparation of original solutions-Classification of cations into analytical groups- Condition for precipitation, application of solubility product and common ion effect in qualitative analysis- Cleaning- Soap reaction with acids and hard water effect of high temperature- Chemistry of cleaning soap micelle cleaning action of soap- Dry cleaning general rules for stain removal chemicals used for spots and stains from fabrics- Synthetic detergent and their advantages over soap- Safety in laboratory- General safety measures (safety equipment, safety notices, personal protection, dangers to avoid)- Chemical hazards (corrosive, irritant substances, toxic compounds, flammable explosives)- Physical hazards (fire, pressure) fire extinguisher- Spillage and waste disposal- First aid (immediate assistance, burns, eye injuries, bleeding, toxic materials) first aid kit

Note: Course materials will be supplied to the students

ALLIED CHEMISTRY PRACTICAL – I (FOR PHYSICS)
Inorganic qualitative analysis
(Subject Code: 21UCHAP31)

Semester:III	**Allied: AP3**	**Credit: 1**	**Hours/W : 2**

Qualitative analysis of a simple salt containing one anion and one cation

ANIONS: Carbonate, Borate, Fluoride, Oxalate and Phosphate

CATIONS: Lead, Bismuth, Copper, Cadmium, Cobalt, Nickel, Manganese, Zinc, Barium, Strontium and Ammonium

Note: Laboratory manual is supplied

ALLIED CHEMISTRY II (FOR PHYSICS)
SUBJECT CODE: 21UCHA41

Semester : IV	Core : 1	Credits : 4	Hours / W : 4

OUTCOME:

- Learning nomenclature of organic compounds
- Development of knowledge in the area of electromotive force
- Understanding various processes involved in metallurgy
- Knowing application of chemistry in industries
- Development in practical knowledge

UNIT I NOMENCLATURE AND ISOMERISM OF ORGANIC COMPOUNDS 12 hrs

Nomenclature of organic compounds - Alkane, alkene, alkyne, cycloalkane and alkyl groups- IUPAC names of alcohols, acids, aldehyde and ketones- Hybridization- Need for the concept of hybridization- sp, sp^2 and sp^3 hybridization with suitable examples- Isomerism in organic compounds- Structural isomerism types with example- Stereoisomerism conformational, geometrical and optical isomerism- Geometrical isomerism cis and trans nomenclature- Optical isomerism elemental of symmetry chirality optical activity- enantiomers, diastereomers,mesomer and racemic mixture optical activity exhibited by lactic acid and tartaric acid

UNIT II ELECTROMOTIVE FORCE 12 hrs

Introduction- Requirements of an electrochemical change- Electrochemical cells difference between electrolytic and galvanic cells- Salt bridge- Electrode potential and standard electrode potential- Electrochemical series and applications- Conventions used in electrode representation and in cell representation- Types of electrodes description of hydrogen, calomel and glass electrodes Nernst equation- Weston cadmium cell- Experimental determination of a cell emf and determination of electrode potential simple calculation- Potentiometric titrations and their advantages principle and method of acid base, redox and precipitation titrations- Determination of pH using hydrogen, glass and quinhydrone electrodes

UNIT III METALLURGICAL PRINCIPLES AND POLYMERS 12 hrs

Minerals and ores- Native,sulphide, oxide, carbonate, halide and sulphate ores- Metallurgy - extraction metals- Concentration of ores hand picking, gravity separation,magnetic separation, froth flotation processes and leaching- Calcination and roasting- Purification of metals electrolysis and zone refining method- Polymers - Properties of polymers ;Mechanical, physical, thermal, optical, electrical and chemical properties- Preparation and uses of thermoplastics polyethylene and PVC- Preparation and uses of thermosetting plastics nylon, epoxy resins, Bakelite- Rubber and uses of rubber- Vulcanization. - Biopolmers

UNIT IV INDUSTRIAL CHEMISTRY AND MAGNETO CHEMISTRY 12 hrs

Silicones preparation, properties and uses- Manufacture and types of glass- Cement composition, manufacture and setting of cement- Fuel gases manufacture, composition and uses of producer gas, water gas, LPG and bio Gas- Softening of water: Ion exchange, electro

dialysis and reverses osmosis methods - Volume, mass and molar susceptibility- Diamagnetism and temperature independent paramagnetism- Temperature dependent paramagetism- Ferro and antiferromagnetism- Measurements of magnetic susceptibility- Applications of magnetic susceptibility studies.

UNIT V PRACTICAL CHEMISTRYII AND SOLVENT EXTRACTION 12 hrs

Introduction definition of various terms (titrations, volumetric analysis, titrant indicator, end point requirements of the reaction selected for the titration commom types of titration. Law of equivalence equivalent weight of acids, bases, oxidizing agents, reducing agents and salts calculation of molecular weights and equivalentweights. Requirements of a primary standard - Secondary standards- Numerical problems in the preparation of solutions- Law of normalities preparation of HCl, H_2SO_4, HNO_3(approximately 0.1N) from standard acids- Principles behind - Acid base titration - pH verses volume curves, choice of indicates form different acid base titrations- Permanganimetry- Dichrometrydiphenylamine and potassium ferricyanide as indicators- Iodimetry Preparation of iodine and starch solutions - starch as indicators- Iodometry role of $KMnO_4$ and $K_2Cr_2O_7$- Solution Nernst distribution law and solvent extraction numerical problems

Note: Course materials will be supplied to the students

ALLIED CHEMISTRY PRACTICAL – II (FOR PHYSICS)
Inorganic qualitative analysis
(Subject Code: 21UCHAP41)

Semester: IV	**Allied: AP4**	**Credit: 1**	**Hours/W: 2**

S. No	Estimation	Link	Standard
1	Strong Acid	Weak Base/Strong Base	Strong Base
2	Strong Acid	Strong Base	Weak Acid
3	Strong Base	Strong Acid	Weak Base
4	Oxalic acid	Potassium Permanganate	Oxalic acid
5	Ferrous Sulphate	Potassium Permanganate	Ferrous Ammonium Sulphate
6	Potassium dichromate	Ferrous Sulphate	Potassium dichromate
7	Ferrous Ammonium Sulphate	Potassium dichromate	Ferrous Sulphate
8	Potassium Permanganate	Sodium thiosulphate	Potassium dichromate
9	Magnesium Sulphate	EDTA	Zinc Sulphate
10	Zinc Sulphate	EDTA	Magnesium Sulphate

Note: Laboratory manual is supplied