

M.Sc. CHEMISTRY

LOCF SYLLABUS 2026



Department of Chemistry

School of Physical Sciences

St. Xavier's College (Autonomous), Palayamkottai

Tirunelveli – 627 002, Tamil Nadu, India

w.e.f. 2026–27

Vision

To mould young men and women as leaders in all walks of life so that they may serve the people especially the poor and the oppressed of our nation in truth, justice and love.

Mission

To achieve a synthesis of academic excellence and the formation of character.

To ensure social justice through equity and access

To include the excluded for empowerment

To equip students with global competencies

To engage in relevant research activities.

To promote Lab to Land through the Outreach Programme – Student Training and Action for Neighbourhood Development (STAND)

SCHOOLS OF EXCELLENCE WITH CHOICE-BASED CREDIT SYSTEM (CBCS)

Essential Features of CBCS

Standardisation of degree courses to internationally accepted levels

Focus on skill-based curriculum

Emphasis on value education

Institution - Industry collaboration

Provision for earning more credits

Development of communication skills

Post Graduate Courses

The existing PG curriculum was thoroughly upgraded based on the expectations of the academicians and the aspirations of the student community. The PG syllabus has two parts : Core and Elective. The minimum number of credits to be earned by a student is 100. The aim of the project work at the PG level is to develop the skill of solving problems and to promote research motivation. All the I-year PG students are offered one Value - Added Course and during their II year they are supposed to do one Extra Credit course outside their class hours to enhance their employability skills. However, during every semester, they are free to learn one ECC paper, offered by the respective departments.

Credit system

The credit system at St. Xavier's College (Autonomous) assigns weightage to courses based on the hours allocated to each course. Typically, one credit is equivalent to one hour of instruction per week. However, credits are awarded regardless of actual teaching hours to ensure consistency and adherence to guidelines. The credits and hours allotted to each course within a programme are detailed in the Programme Pattern table. While the table provides a framework, there may be some flexibility due to practical sessions, field visits, tutorials, and the nature of project work. For postgraduate (PG) courses, students are required to accumulate

a minimum of 100 credits, as stipulated in the programme pattern table. The total number of courses offered by the department is outlined in the Programme Structure.

OUTCOME-BASED EDUCATION (OBE)

Outcome-Based Education (OBE) is a student-centric teaching and learning methodology that focuses on measuring student performance through clearly defined outcomes. For St. Xavier's College, with its commitment to excellence and NAAC/NBA accreditation requirements, OBE is not just a regulatory expectation but a pathway to academic quality, global competitiveness, and improved employability of graduates.

We prepare students to meet future industry requirements and reinforce St. Xavier's College, Palayamkottai, as a leader in quality higher education. St. Xavier's College introduced OBE in 2018, and for the Attainment Calculation, we developed our own method in 2018. From the academic year 2025-26 onwards, in examinations, for each question we mark Course Outcome (CO), Competency and Performance Indicator, Programme Outcome / Programme Specific Outcome, Bloom's Revised Cognitive Level and we follow the OBE procedure for the calculation of the Attainment of Outcome for each student, course, semester, programme.

EVALUATION PATTERN (PG)

Continuous Internal Assessment

There is no internal minimum for any paper. However, Continuous Internal Assessment (CIA) is a mandatory requirement for all students. A student must take at least one CIA test out of two tests and must fulfil at least one mode of assessment among assignments, quiz, seminars, etc., otherwise he/she will not be permitted to write the semester examination.

S.No	Component	Marks Allotted
1	I CIA Test	70
2	II CIA Test	70
	Total	140

The total CIA marks of 140 will be converted to 70 marks. An additional 30 marks will be awarded through other internal assessment components.

The Continuous Internal Assessment (CIA) consists of two component tests, each carrying 15 marks (15 + 15).

The final internal assessment marks will be calculated out of 100 (70 + 30). The obtained marks will be **converted to 50 marks**.

Semester (External) Examination

- The External Semester Examination will be conducted for **100 marks**.
- The obtained marks will be **converted to 50 marks**.

Question Pattern

PG Semester Examinations (3 Hours)

PART	TYPE	Mark Distribution	Total Marks
A	MCQ	10X1	10
B	ALL	5X3	15
C	Either/or	5X6	30
D	3 out of 5	3X15	45
		Total	100

PG Internal Examinations (2 Hours)

PART	TYPE	Mark Distribution	Total Marks
A	MCQ	10X1	10
B	ALL	3X3	09
C	Either/or	3x7	21
D	3 out of 5	3X10	30
		Total	70

Grading System

Range of Marks	Letter Grade	Grade Point	Description
90-100	A+	9.0-10.0	Outstanding
80-89	A	8.0-8.9	Excellent
70-79	B+	7.0-7.9	Very Good
60-69	B	6.0-6.9	Good
50-59	U	5.0-5.9	Average
00-49	U	0	Reappear

PROGRAMME OUTCOMES (PO)

Students of the postgraduate programme in chemistry, at the time of graduation, will be able to attain the following programme outcomes (POs):

PO1.Critical thinking: Acquire the knowledge in the respective field and take informed actions

PO2. Effective communication: Speak, read, write and listen clearly in person and through electronic media in English and in one Indian language, and make meaning of the world by connecting people, ideas, books, media and technology.

PO3.Social interaction: Apply reasoning informed by the contextual knowledge to assess societal, health, safety, legal and cultural issues and the consequent responsibilities relevant to the professional practice.

PO4. Effective Citizenship: Demonstrate empathic social concern and equity centered national development, and the ability to act with an informed awareness of issues and participate in civic life through volunteering.

PO5. Ethics: Recognize different values systems and apply ethical principles and commit to professional ethics and responsibilities and norms of different value systems.

PO6. Environment and Sustainability: Demonstrate the issues of environmental contexts and sustainable development.

PO7. Modern tool usage: Create, select, and apply appropriate techniques, resources, and modern IT Tools including prediction and modeling to complex activities with an understanding of the limitations.

PO8. Self-directed and lifelong Learning: Recognize the need for and have the preparation and ability to engage in independent and life-long learning in the broadest context of socio-technological changes.

PROGRAMME SPECIFIC OUTCOMES (PSO)

PSO1. Advanced Chemical Knowledge: Apply indepth knowledge on advanced concepts in Organic, Inorganic, Physical, Analytical, Biological, Environmental and Industrial chemistry in research based endeavours with practical applications to address complex scientific problems.

PSO2. Experimental and Laboratory Skills: Design and perform advanced laboratory experiments, employing standard operating procedures, modern instrumentation, and safe laboratory practices to obtain accurate and reproducible results.

PSO3. Analytical and Spectroscopic Instrumentation: Apply advanced analytical and spectroscopic techniques such as UV-Visible, FT-IR, NMR, Mass Spectrometry, HPLC, GC, and XRD for qualitative and quantitative analysis of chemical substances.

PSO4. Professional Development and Entrepreneurship: To make current awareness on social, economic, and environmental problems facing globally and motivate the students to prepare for competitive examinations and get trained for industrial entrepreneurship.

PSO5. Computational Chemistry and Data Analysis: Utilize computational chemistry, molecular modeling, chemoinformatics, statistical tools, ICT tools and scientific software for data analysis, molecular simulations, and predictive studies. .

PSO6. Scientific Reasoning, Critical Thinking, and Problem Solving: Analyze complex chemical problems using scientific reasoning, critical thinking, and interdisciplinary approaches to develop effective and sustainable solutions.

PSO7. Industrial Applications and Regulatory Compliance: Apply chemical knowledge in pharmaceuticals, materials science, environmental monitoring, food technology, energy, and chemical industries while considering quality standards and regulatory requirements.

PSO8. Professional Ethics, Safety, and Sustainable Practices: Demonstrate ethical conduct, environmental awareness, laboratory safety, and responsible handling of chemicals, ensuring sustainable practices in research and industrial settings.

Sem	Part	Status	Sub. Code	Title of the paper	Hr	Cdt
I	A	Core-1	26PCHC11	Organic Chemistry-I	6	5
		Core-2	26PCHC12	Inorganic Chemistry -I	6	5
		Core-3	26PCHC13	Organic Chemistry Practical -I	4	2
		Core-4	26PCHC14	Inorganic Chemistry Practical -I	4	2
	B	EC-1	26PCHE11	Nano and Supramolecular Chemistry	5	3
		EC-2	26PCHE12	Molecular Spectroscopy	5	3
					30	20
II	A	Core-5	26PCHC21	Organic Chemistry-II	5	5
		Core-6	26PCHC22	Physical Chemistry -I	5	5
		Core-7	26PCHC23	Organic Chemistry Practical -II	4	2
		Core-8	26PCHC24	Inorganic Chemistry Practical-II	4	2
	B	EC-3	26PCHE21	Selected Topics in Inorganic Chemistry	4	3
		EC-4	26PCHE22	Medicinal Chemistry	4	3
		SEC-1	26PCHS21	Analytical and Green Chemistry	4	2
	C	Extension Activities	-	STAND (Student Training and Action for Neighbourhood Development)	-	1
					30	23
III	A	Core-9	26PCHC31	Organic Chemistry-III	5	5
		Core-10	26PCHC32	Inorganic Chemistry-II	5	5
		Core-11	26PCHC33	Physical Chemistry -II	5	5
		Core-12	26PCHC34	Physical Chemistry Practical- I	4	2
		Core-13	26PCHC35	Analytical Instrumentation Technique Practicals	4	2
	B	EC-5	26PCHE31	Biomolecules and Heterocyclic compounds	4	3
		SEC-2	26PCHS31	Research Methodology and Cheminformatics	3	2
		Internship	26PCHI35	Carried out in summer vacation at the end of Sem II	-	2
					30	26
IV	A	Core-14	26PCHC41	Inorganic Chemistry-III	6	5
		Core-15	26PCHC42	Physical Chemistry-III	6	5
		Project	26PCHC43	Project with Viva Voce	10	7
	B	EC-6	26PCHE41	Physical Chemistry Practical-II	4	3
		SEC-3	26PCHS41	Training for competitive Examination	4	2
					30	22
					120	91

	Value Added Course	26PCHVA1	Fundamentals in Phytochemistry	-	3
	Extra Credit Course	26PCHEC1	Chemistry in Consumer Products	-	3
		26PCHEC2	Forensic Chemistry		
		26PCHEC3	Health Chemistry		
		26PCHEC4	Environmental Chemistry		
				MOOC	2
				Field Visit	1
				120	100

Abbreviation

C- Core

SEC- Skill Enhancement Course

EC- Elective Course

I- Internship

ORGANIC CHEMISTRY– I

(26PCHC11)

Semester-I Core-1 Hours/W: 6 Credits: 5

Course Outcomes:

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

CO1: Recall the basic principles of organic reactions, reagents and stereochemistry (K1)

CO2: Describe the reaction intermediates, symmetry, chirality, racemization and role of reagents in organic chemistry. (K2)

CO3: Apply the principles of reaction mechanism, different types of reagents and stereochemistry in various organic reactions (K3)

CO4: Analyse the mechanism and stereochemistry of nucleophilic and electrophilic substitution reactions with the aid of different types of reagents (K4)

CO5: Justify the suitable reaction mechanism and reagents for organic reactions and stereochemistry of organic compounds (K5)

CO6: Design a template to correlate the reaction mechanism, stereochemistry and reagents for common organic reactions. (K6)

UNIT-I: Methods of Determination of Reaction Mechanism (18 Hrs)

Reaction intermediates, The transition state, reaction coordinate diagrams, and thermodynamic and kinetic requirements of reactions: Hammond postulate and Curtin-Hammett Principle. Methods of determining mechanism: non-kinetic methods—product analysis, determination of intermediates, isolation, detection, and trapping. Cross-over experiments, isotopic labeling, isotope effects, and stereochemical evidence. Kinetic methods—relation of rate and mechanism. Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship.

Self-Study: ^{18}O -labeled water to study ester hydrolysis

UNIT-II: Aromatic and Aliphatic Electrophilic Substitution (18 Hrs)

Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds, and annulenes. Aromatic electrophilic substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene, and halobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling; Sulfur electrophiles: sulfonation; halogen electrophiles: chlorination and bromination; carbon electrophiles: Friedel-Crafts alkylation, acylation, and arylation reactions. Aliphatic electrophilic substitution mechanisms: $\text{S}_{\text{E}}2$ and $\text{S}_{\text{E}}\text{i}$, $\text{S}_{\text{E}}1$ -mechanism, and evidences.

Self-Study: Factors governing selectivity and reactivity.

UNIT-III: Aromatic and Aliphatic Nucleophilic Substitution

(18 Hrs)

Aromatic nucleophilic substitution: Mechanisms - S_NAr , S_N1 and Benzyne mechanisms - Evidences - Reactivity, Effect of structure, leaving group and attacking nucleophile. S_N1 , ion pair, S_N2 mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon. S_N1 , S_N2 , S_Ni , mechanism and evidences. 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)

Self-Study: Photochemical S_NAr reactions.

UNIT-IV: Stereochemistry-I

(18 Hrs)

Stereochemistry- Concept of chirality, Chirality - Prochiral centre, Prochiral face, Homotopic, Enantiotopic and diastereotopic ligands. Optical isomerism due to asymmetric and dissymmetric molecules with C and N based chiral centres. Racemic modifications: Racemization by epimerization and mutarotation. D, L system, Cram's and Prelog's rules: R, S-notations, proR, proS, side phase and re-phase, Cahn-Ingold- Prelog rules, absolute and relative configurations. Configurations of allenes, spiranes, biphenyls, binaphthyls. Topicity and pro-stereoisomerism, chiral shift reagents and chiral solvating reagents. Asymmetric synthesis. Stereoselective and stereospecific synthesis.

Self-Study: Chiral HPLC, GC, and capillary electrophoresis

Unit-V: Stereochemistry-II

(18 hrs)

Conformation and reactivity of acyclic systems, intramolecular rearrangements, and neighbouring group participation. Stability of five and six-membered rings: mono and disubstituted cyclohexanes, conformation and reactivity in cyclohexane systems. Fused and bridged rings: bicyclic- cis & trans decalins and Brett's rule. Optical rotation and optical rotatory dispersion, conformational asymmetry, CD and ORD curves, octant rule, configuration and conformation, Cotton effect, axial haloketone rule and determination of configuration.

Self-Study: Anomeric effect.

Text Books:

1. J. March and M. Smith, Advanced Organic Chemistry, 5th edition, John-Wiley and Sons.2001.
2. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
3. P.S.Kalsi, Stereochemistry of carbon compounds, 8th edition, New Age International Publishers, 2015.

4. P. Y. Bruice, Organic Chemistry, 7th edn., Prentice Hall, 2013.
5. J. Clayden, N. Greeves, S. Warren, Organic Compounds, 2nd edition, Oxford University Press, 2014.

Reference Books:

1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part-A and B, 5th edition, Kluwer Academic / Plenum Publishers, 2007.
2. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001.
3. N.S. Isaacs, Physical Organic Chemistry, ELBS, Longman, UK, 1987.
4. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata-McGraw Hill, 2000.
5. I. L. Finar, Organic chemistry, Vol-1 & 2, 6th edition, Pearson Education Asia, 2004.

INORGANIC CHEMISTRY-I

(26PCHC12)

Semester-I

Core-2

Hours/W: 6

Credits: 5

Course Outcomes:

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

CO1: Recall the simple laws and principles involved in solid state chemistry (K1)

CO2: Summarize the fundamental principles of crystallography, crystal structures, acid–base theories, ionic and covalent bonding concepts (K2)

CO3: Apply the concepts of X-ray diffraction, band theory, lattice energy calculations and VSEPR theory to solve structural and bonding problems (K3)

CO4: Analyze crystal defects, electronic structure of solids, acid–base behavior -HSAB concept and MO configurations of diatomic and polyatomic molecules (K4)

CO5: Evaluate molecular geometry, bond strength, stability, and reactivity using MO theory, Bent's rule, Berry pseudorotation, and acid–base strength parameters (K5)

CO6: Construct MO diagrams, Born–Haber cycles, and predict structures and properties of inorganic compounds using integrated bonding and structural concepts (K6)

Unit I: Solid State Chemistry – I

18 hrs

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. AX₂ type - Rutile, fluorite, antiferite. ABX₃ type- Perovskite, AX₃ type- ReO₃. Covalent crystals – diamond, graphite and fullerenes

Self-Study: Close packing of solids

Unit II: Solid State Chemistry – II

18 hrs

Crystal defects- Line defect, plane 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

18 hrs

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

18 hrs

Ionic bond and its characteristic features-Lattice energy, Born-Landé equation, Born Haber cycle and its applications (NaCl , KCl , MgBr_2). Radius ratio rule and its applications - Polarization- Fajan's rule - 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

18 hrs

Valence bond theory - Resonance- Formal charge. Hybridisation and Overlap. MO theory-Symmetry and overlap. Molecular Orbitals in homonuclear diatomic molecules - B_2 , C_2 , N_2 , O_2 and F_2 . MO of heteronuclear diatomic molecules - CO and HCl . MO of triatomic molecule – BeH_2 . MO of polyatomic molecules- NH_3 . VSEPR Theory and its applications- CO_2 , $\text{B}(\text{CH}_3)_3$, COCl_2 , POF_3 , PF_5 , SF_6 , $[\text{NH}_4]^+[\text{BF}_4]^-$, 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 , CH_3F , H_2O and SF_4) and the energetics of hybridization. Berry pseudorotation- PF_5 .

Self-Study: Hydrates and Clathrates

Text Books:

1. A R West, Solid state Chemistry and its applications, 2nd Edition (Students Edition), John Wiley & Sons Ltd., 2014.
2. L Smart, E Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2012.
3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry; W.B. Saunders company: Philadelphia, 1977.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: New York, 1983.

Reference Books:

1. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994.
2. C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2nd

Edition, Cambridge University Press, 1991.

3. T. Moeller, Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982.
4. D. F. Shriver, P. W. Atkins and C.H. Langford; Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.
5. L. Azaroff, "Introduction to Solids", 3rd edition, 1977, Tata Mc-Graw Hill.
6. M.G. Arora, Solid state chemistry, 2001, Anmol Publication Pvt. Ltd., New Delhi.
7. Addison. W.E., Structural principles of Inorganic chemistry, 1961, Willey Interscience, New York.
8. Sisler, Chemistry in non – aqueous solvents, 1961, Reinhold publishing Corporation.

ORGANIC CHEMISTRY PRACTICAL-I

(26PCHC13)

Semester-I

Core-3

Hours/W: 4

Credits: 2

Course Outcomes:

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

CO1: List the underlying principle of separation, micro scale qualitative analysis and synthesis of organic compounds (K1)

CO2: Restate the separation, preparation and synthesis of organic compounds (K2)

CO3: Apply the analytical skill in identifying the functional groups in the organic compounds (K3)

CO4: Outline the techniques involved in single step organic synthesis (K4)

CO5: Assess the suitable techniques for separation, analysis and synthesis (K5)

CO6: Develop the skill in separation, qualitative analysis, synthesis and recrystallization techniques (K6)

UNIT-I: Separation and analysis

A. Two component mixtures. B. Three component mixtures.

Unit-II Preparation of Organic Compound (Single Stage)

- i) Oxidation of toluene to benzoic acid
- ii) Bromination of Acetanilide
- iii) Nitration of phenol
- iv) Glucosazone
- v) Methyl orange dye
- vi) Methyl red dye

Text Books:

1. Gnanapragasam. N.S., Ramamurthy. G., Organic Chemistry Lab Manuel, S. Viswanathan Pvt. Ltd.

Reference Books:

1. Furniss, Hannaford, Smith, Tatchell, Vogel's textbook of Practical Organic Chemistry, Pearson education.

INORGANIC CHEMISTRY PRACTICAL-I

(26PCHC14)

Semester-I

CORE-4

Hours/W: 4

Credits: 2

Course Outcomes:

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

CO1: List the aim and principles of semi micro qualitative and complexometric analysis (K1)

CO2: Outline the procedure for Inorganic qualitative and complexometric analysis (K2)

CO3: Identify the ions, and apply the complexometric titration using EDTA method (K3)

CO4 : Detect the cations into the groups, mask the selective ions with suitable agents (K4)

CO5: Estimate the analytes using complexometric titration using EDTA by direct and indirect methods (K5)

CO6 : Formulate new techniques for complexometric titration using masking agents (K6)

UNIT-I: Analysis of mixture of cations

Analysis of a mixture of four cations containing two common cations and two rare cations. Cations to be tested.

Group-I : W, Tl and Pb.

Group-IA : Se and Te

Group-II : Mo, Cu, Bi and Cd.

Group-III : Tl, Ce, Th, Zr, V, Cr, Fe, Ti and U.

Group-IV : Ni, Co, Zn and Mn.

Group-V : Ba, Ca and Sr.

Group-VI : Li and Mg.

UNIT-II: Complexometric Titration

1. Estimation of Zinc, Nickel, Magnesium, Copper and Calcium.

2. Estimation of mixture of metal ions-pH control, masking and demasking agents.

Text Books:

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rdedn., The National Publishing Company, Chennai, 1974.

2. G. Svehla, Vogel's Text book of Macro and Semimicro Qualitative Inorganic Analysis, 5thedn., Longman, London and New York.

3. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, "Vogel's Text book of Inorganic Quantitative Analysis", 5thed., Longman Scientific & Technical, New York.

Reference books:

- . 1. G. Pass, and H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965.
2. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954.

NANO AND SUPRAMOLECULAR CHEMISTRY

(26PCHE11)

Semester-I

EC-1

Hours/W: 5

Credits: 3

Course Outcomes:

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

CO1: Recognize the methods of fabricating nanostructures and concepts of supramolecular chemistry (K1).

CO2: Relate the properties of nanomaterials to reduce dimensionality of the material (K2).

CO3: Organize the tools for properties of nanostructures and dendrimers. (K3).

CO4: Illustrate the applications of nanomaterials and supramolecules (K4).

CO5: Appraise the characters of various nano materials synthesized by new technologies (K5).

CO6: Design synthetic routes for new nanomaterials and supramolecular assemblies (K6).

UNIT-I: Introduction of nanomaterials (15 Hrs)

Introduction-role of size, classification-0D, 1D, 2D, 3D. Synthesis-Bottom –Up, Top–Down, consolidation of Nano powders. Features of nanostructures, Background of nanostructures. Techniques of synthesis of nanomaterials, Tools of the nanoscience. Applications of nanomaterials and technologies.

Self-Study: Nano reactors

UNIT-II: Synthesis and characterization of Nanomaterials (15 Hrs)

Synthesis- Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvothermal and hydrothermal-CVD-types, metallo organic, plasma enhanced, and low-pressure CVD. Microwave assisted and electrochemical synthesis. Characterization – SEM, TEM and AFM - principle, instrumentation and applications.

Self-Study: Lithography

UNIT-III: Properties of Nanomaterials (15 Hrs)

Mechanical properties of materials, theories relevant to mechanical properties. Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials Nanoparticles: gold and silver, metal oxides: silica, iron oxide and alumina - synthesis and properties.

Self-Study: Superparamagnetism

Unit IV: Supramolecular Chemistry (15 Hrs)

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

(15 Hrs)

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: Molecular necklaces, Allosteric Switch.

Text Books:

1. S. Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications, 2007.
3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010.
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.
5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th edn., Pearson Press, 2007.
6. J.W. Steed, J.L. Atwood, Supramolecular chemistry, 2000, John Willey & sons Ltd. New York.

Reference Books:

1. S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016.
2. Arumugam, Materials Science, Anuradha Publications, 2007.
3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010
4. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.
5. J. M. Lehn, Supramolecular Chemistry, Concepts and perspectives, 1995, VCH; Weinheim.

MOLECULAR SPECTROSCOPY

(26PCHE12)

Semester-I

EC-2

Hours/W: 5

Credits: 3

Course Outcomes:

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

CO1: Recall fundamental principles of rotational, Raman, IR, electronic, Mössbauer, NMR, ESR, XPES and NQR spectroscopy (K1).

CO2: Explain rotational and vibrational energy levels and spectral transitions (K2).

CO3: Describe electronic spectra, Franck–Condon principle and Mössbauer parameters (K3).

CO4: Interpret Mössbauer, XPES and NQR spectral parameters (K4).

CO5: Evaluate suitability of different spectroscopic techniques for structural analysis (K5).

CO6: Integrate IR, Raman, NMR, ESR and electronic spectra for structure elucidation (K6).

UNIT-I: Rotational and Raman Spectroscopy (15 Hrs)

Rotation of molecules on the basis of moments of Inertia: Spherical-Top, symmetric, asymmetric & linear. Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators. Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, Stokes and anti-Stokes lines. Vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, Polarization of Raman scattered photons.

Self-Study: Depolarization ratio

UNIT-II: Vibrational Spectroscopy (15 Hrs)

Infra-red spectroscopy – review of linear harmonic oscillator – vibrational energies of diatomic molecules – selection rule – Zero point energy, dissociation energy, force constant and bond strength – 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 FT-IR.

Self-Study: Isotopic Frequency Shifts

UNIT-III: Electronic and Mossbauer Spectroscopy (15 Hrs)

Electronic spectra of diatomic molecules- vibrational coarse structure, Frank-Condon principle: Intensity of vibrational – electronic spectra, dissociation energy, dissociation products, rotational fine structure of electronic –vibrational transitions.

Mossbauer spectroscopy -. Principle, Doppler shift, Recoil energy – Isomer shift – Quadrupole splitting – Hyperfine splitting – applications to various compounds.

Self study: Nordheim's rule

UNIT-IV: PES and NQR spectroscopy (15 Hrs)

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

Self-Study: Nuclear Quadrupole Moment

UNIT-V: NMR and ESR Spectroscopy (15 Hrs)

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 absorptions – anisotropy in g-value – fine splitting - hyperfine splitting in ESR – zero field splitting, Kramer's rule – calculation of electron density in radicals.

Self study: McConnell equation

Text Books:

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata McGraw Hill, New Delhi, 2000.
2. R. M. Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th Ed., John Wiley & Sons, New York, 2003.
3. W. Kemp, Applications of Spectroscopy, English Language Book Society, 1987.
4. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1992.

Reference Books:

1. P.W. Atkins and J. de Paula, Physical Chemistry, 7th Ed., Oxford University Press, Oxford, 2002.
2. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons, New York, 1974.
3. A. Rahman, Nuclear Magnetic Resonance-Basic Principles, Springer-Verlag, New York, 1986.

4. K. Nakamoto, Infrared and Raman Spectra of Inorganic and coordination Compounds, Part-B: 5th ed., John Wiley& Sons Inc., New York, 1997.
5. J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance; Wiley Interscience, 1994.

ORGANIC CHEMISTRY-II

(26PCHC21)

Semester-II

CORE-5

Hours/W: 5

Credits: 5

Course Outcomes:

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

CO1: Recall principles of retrosynthetic analysis, synthons and synthetic equivalents (K1)

CO2: Explain mechanisms and stereochemistry of elimination reactions (K2)

CO3: Apply elimination mechanisms to predict products and stereochemistry (K3)

CO4: Analyze photochemical rearrangements and reaction pathways (K4)

CO5: Evaluate stereochemical assignments using ORD/CD and octant rule (K5)

CO6: Develop pericyclic reaction strategies in organic synthesis (K6)

UNIT-I: Retrosynthetic Analysis

(15 Hrs)

Retrosynthetic analysis - Examples on retrosynthetic approach, calculation of yield. Planning of synthesis – Guidelines and rules for Disconnection approach, Synthons and synthetic equivalents, Synthon Approach-Nucleophiles and electrophiles. Functional group addition. Synthesis of organic mono and bifunctional compounds via disconnection approach. One group disconnection- alcohol, ketones and acids. Two group disconnection: 1,2-, 1,3- and 1,4- difunctional compounds. convergent synthesis and divergent synthesis. Synthesis based on umpolung concepts of Seebach. Protection and deprotection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Functional group interconversion.

Self-Study: Functional group addition.

UNIT-II: Elimination Reactions

(15 Hrs)

Mechanisms: E2, E1, and E1CB mechanisms. Syn- and anti-eliminations. Orientation of the double bond: Hoffmann and Saytzeff rules- Chugaev reaction, Cope reactions. Reactivity: Effect of substrate, attacking bases, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems, pyrolytic elimination.

Self-Study: Factors affecting elimination reaction.

Unit-III: 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: DIBAL-H, Tri-n-butyltin hydride, Baker yeast. Phase transfer catalysts, crown ether, LDA, $(\text{CH}_3)_3\text{SiI}$, Aluminiumisopropoxide, diazomethane, Organo rhodium compounds. AIBN, Gilman reagent, Merrifield resin, Collin's reagent, 1,3 dithiane and CAN.

Self-Study: Swern reagent

UNIT-IV: 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, Di π -methane rearrangement, Photo oxidation-Barton reaction. Photoaddition: Photoaddition of alkene to carbonyl compounds-Photoaddition of alkenes and alkynes to aromatic compounds. Photochemistry of α,β -unsaturated ketones. Photochemistry of aromatic compounds, Photo-Fries rearrangement.

Self-Study: photoisomerization of rhodopsin in the retina

UNIT-V: Pericyclic Reactions**(15 Hrs)**

Pericyclic reactions - Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5- hexatriene and allyl system. Classification of pericyclic reactions Woodward-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 antarafacial additions; $4n$ and $4n+2$ system. Sigmatropic reactions - Woodward-Hoffmann rule and FMO method - Suprafacial and antarafacial shifts of Hydrogen - Sigmatropic shifts in moving carbon moieties. 1,3-, 1,5- and 3,3-sigmatropic 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: Chelotropic Reactions

Text Books:

1. J. March and M. Smith, Advanced Organic Chemistry, 5th ed., John-Wiley and Sons. 2001.
2. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
3. P. S. Kalsi, Stereochemistry of carbon compounds, 8thedn, New Age International Publishers, 2015.
4. P. Y. Bruice, Organic Chemistry, 7thedn., Prentice Hall, 2013.
5. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee Organic Chemistry, 7th edn., Pearson Education, 2010.
6. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001.
7. P. S. Kalsi, Stereochemistry of carbon compounds, 8th edition, New Age International Publishers, 2015.
8. Gill and Wills, Pericyclic Reactions, Chapman Hall, London, 1974.

References:

1. Stuart Warren and Paul Wyatt, Organic Synthesis-The Disconnection Approach, Wiley, 2nd edn.,
2. S. H. Pine, Organic Chemistry, 5th edn, McGraw Hill International Edition, 1987.
4. L. F. Fieser and M. Fieser, Organic Chemistry, Asia Publishing House, Bombay, 2000.
3. E.S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959.
4. T. L. Gilchrist, Heterocyclic Chemistry, Longman Press, 1989.
5. J. A. Joule and K. Mills, Heterocyclic Chemistry, 4th ed., John-Wiley, 2010.

PHYSICAL CHEMISTRY-I

(26PCHC22)

Semester-II

Core-6

Hours/W: 5

Credits: 5

Course Outcomes:

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

CO1: Know The Importance Of Quantum Mechanical Models Of Particle In a Box, Rigid Rotor And Harmonic Oscillator (K1).

CO2: Understand The Essential Characteristics Of Wave Functions And Need For The Quantum Mechanics (K2).

CO3: Apply The Quantum Mechanics To Hydrogen And Polyelectronic Systems (K3).

CO4: Familiarize the Symmetry In Molecules And Predict The Point Groups (K4).

CO5: Justify The Characteristics Of Wave Functions And Symmetry Functions (K5).

CO6: Predict The Vibrational Modes, Hybridization Using Helium Concepts of Group Theory (K6).

UNIT-I: Quantum Chemistry

(15 Hrs)

Inadequacy of Classical mechanics and dawn of Quantum chemistry: Black - body radiation and photoelectric effect. Wave function and its significance – eigenfunctions and eigenvalues – orthogonality and normalization. Schrodinger time independent wave equation, Postulates of quantum mechanics -- different types of functions. Quantum mechanical operators – position operator, linear momentum operator, angular momentum operator, kinetic energy operator and Hamiltonian operator and Hermitian operator – commutation relationship among L_x , L_y , L_z and L^2 operators. Setting up Schrodinger equation, solution & interpretation with regard to particle in a 1 –D box and 3 – D box. Schrödinger equation for electron in a ring, rigid rotor and simple harmonic oscillator.

Self-Study: Anharmonic oscillator concept.

UNIT-II: Applications of Quantum Chemistry-I

(15 Hrs)

Setting up Schrodinger equation for H – atom, separation into three equations (without derivation), quantum numbers and their importance. Approximation methods – Need for approximation, Perturbation theory – Time independent Perturbation (First order only), Application of perturbation theory to particle in one dimensional box and anharmonic oscillator. Principle of variation method and its proof. Variation methods and its applications to hydrogen atom and helium atom.

Self-Study: Self-consistent field approximation.

UNIT-III: Applications of Quantum Chemistry-II**(15 Hrs)**

Hartree-Fock self-consistent method, quantum mechanical tunneling and experimental evidence of quantum mechanical tunneling. Pauli's exclusion principle and Slater determination. The Born-Oppenheimer approximation, MO & VB theories as applied to the 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, Slater type orbitals. Huckel molecular orbital theory – principles, applications and calculations of pi electron energies to ethylene and butadiene.

Self-Study: calculations of pi electron energies to benzene.

UNIT-IV: Group theory**(15 Hrs)**

Groups, sub groups, symmetry elements, operations, classification-axial and non-axial. Dihedral point groups- C_n , C_{nh} , D_n , D_{nh} , D_{nd} , T_d and O_h . Matrix representation and classes of symmetry operations, reducible irreducible and direct product representation. The Great orthogonality theorem – irreducible representation and reduction formula, construction of character table for C_{2v} , C_{2h} , C_{3v} and D_{2h} point groups.

Self-Study: Vibrational mode analysis of polyatomic molecules.

UNIT-V: Applications of group theory**(15 Hrs)**

Standard reduction formula, Group Theory (GT) applied to determine hybridization scheme in CH_4 and BF_3 . Application of GT to normal mode analysis of $[PtCl_4]^{2-}$, H_2O , NH_3 and BF_3 and CO_2 . Symmetry properties of integrals and symmetry – based selection rule for vibrational spectra – Identification of IR and Raman active fundamentals. Selection rule for electronic transition – prediction of electronic transitions in formaldehyde. – Application of GT to trans – 1, 3 – butadiene and benzene- calculations and delocalization energy in trans – 1, 3 – butadiene and benzene.

Self-Study: Symmetry treatment of aromatic and antiaromatic systems.

Text Books:

1. R.K. Prasad, Quantum Chemistry, New Age International Publishers, New Delhi, 2010, 4th revised edition.
2. F. A. Cotton, Chemical Applications of Group Theory, John Wiley & Sons, 2003, 2nd edition.
3. Vincent, Molecular Symmetry and Group Theory. A Programmed Introduction to Chemical Applications, John and Willy & Sons Ltd., 2013, 2nd Edition.
4. T. Engel & Philip Reid, Quantum Chemistry and Spectroscopy, Pearson, New Delhi, 2018, 4th edition.
5. G. K. Vemulapalli, Physical Chemistry, Prentice Hall of India Pvt. Ltd. 2001.
6. D.A. McQuarrie, Quantum Chemistry, Viva Books PW. Ltd, 2013, 2nd edition.

Reference Books:

1. N. Levine, Quantum Chemistry, Allyn& Bacon Inc, 1983, 4th edition.
2. D.A. McQuarrie and J. D. Simon, Physical Chemistry, A Molecular Approach, Viva Books Pvt. Ltd, New Delhi, 2012.
3. R. P. Rastogi & V. K. Srivastava, An Introduction to Quantum Mechanics of Chemical
4. Systems, Oxford & IBH Publishing Co., New Delhi, 1999.
5. R.L. Flurry. Jr, Symmetry Group Theory and Chemical applications, Prentice Hall. Inc, 1980
6. J. M. Hollas, Symmetry in Molecules, Chapman and Hall, London, 2011, Reprint

ORGANIC CHEMISTRY PRACTICAL-II

(26PCHC14)

Semester-II

Core-7

Hours/W: 4

Credits: 2

Course Outcomes:

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

CO1: Recall the principle underlying estimations of organic compounds (K1)

CO2: Interpret the reactions of estimated organic compounds (K2)

CO3: Examine the organic compounds in the research laboratories and industry(K3)

CO4: Analyse the organic compounds quantitatively through standard procedures (K4)

CO5: Classify the organic compounds based on synthetic routes and estimation method (K5)

CO6: Formulate a template to interconnect the quantitative analysis and synthetic method of organic compounds (K6)

UNIT-I: Estimations

- a) Estimation of Phenol (bromination)
- b) Estimation of Aniline (bromination)
- c) Estimation of Glucose (redox)
- d) Estimation of Ascorbic acid (iodimetry)
- e) Estimation of Glycine (acidimetry)
- f) Estimation of Formalin (iodimetry)

UNIT-II: Two stage preparations

- a) p-bromoacetanilide from aniline
- b) p-nitroaniline from acetanilide
- c) 1,3,5-Tribromobenzene from aniline
- d) Acetylsalicylic acid from methyl salicylate
- e) Benzilic acid from benzoin

Text Book:

1. Gnanapragasam. N.S., Ramamurthy. G., Organic Chemistry Lab Manuel, S. Viswanathan Pvt.Ltd.

Reference Book:

1. Furniss, Hannaford, Smith, Tatchell, Vogel's textbook of Practical Organic Chemistry, Pearson education.

INORGANIC CHEMISTRY PRACTICAL-II

(26PCHC24)

Semester-II

CORE-8

Hours/W: 4

Credits: 2

Course Outcomes:

CO1: List the aim and principles of Quantitative analysis and complex preparation (K1)

CO2: Outline the procedure for Inorganic quantitative analysis and complex preparations

CO3: Quantify the ions, and apply the Gravimetric and volumetric titration methods

CO4: Analyse the ions present in the mixture and measure them quantitatively

CO5: Estimate the analytes using gravimetric titration methods

CO6: Formulate new techniques for gravimetric titration using masking agents and Inorganic complex preparation .

UNIT-I: 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)

UNIT-II: Preparation of metal complexes

Preparation of Inorganic complexes:

- a. Preparation of trithiourea copper (I) sulphate
- b. Preparation of potassium trioxalatochromate(III)
- c. Preparation of tetrammine copper(II) sulphate
- d. Preparation of hexathiourea copper(I) chloridedihydrate
- e. Preparation of sodium trioxalato ferrate(III)
- f. Preparation of hexathiourea lead(II) nitrate

Text Books

1. Vogel's Text book of Inorganic Quantitative Analysis, 4thed., ELBS, London.
2. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, "Vogel's Text book of Inorganic Quantitative Analysis", 5thedn., Longman Scientific & Technical, New York.

Reference books

1. G. Pass, and H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965.
2. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954

SELECTED TOPICS IN INORGANIC CHEMISTRY

(Subject code: 26PCHE21)

Semester-II

EC-3

Hours/W: 4

Credits: 3

COURSE OUTCOMES:

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

CO 1: Recalls the comprehensive knowledge of inorganic chemistry, bioinorganic systems, medicinal inorganic chemistry, enzyme chemistry, and selected inorganic compounds (K1)

CO 2: Explain the biochemical roles of metals and non-metals, metal toxicity, role of heme and non-heme proteins (K2)

CO 3: Apply the mechanistic principles to ion transport, metalloenzymes and metal-based drugs (K3)

CO 4: Organise the structure–function relationships in enzymes, medicinal agents, zeolites, spinels and nanomaterials (K4)

CO 5: Evaluate synthetic strategies, catalytic mechanisms and therapeutic effectiveness of inorganic compounds (K5)

CO 6: Design advanced bioinorganic models, reaction mechanisms and functional materials for environmental and biomedical applications (K6)

Unit- I: Pollution and Toxic effects of trace elements

(12 hrs)

Trace metals like Pb, Cd, As, Hg - Toxicity, Impact of poisoning, prevention and remedies. Fluoride contamination-Source, strategies to tackle fluoride contamination. NO poisoning. Ozone layer- cause and effect of ozone depletion, preventive measures. CFCs- source and impact.

Self-Study: Acid rain and Smog

Unit- II: Biochemistry of metals and non-metals

(12 hrs)

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

(12 hrs)

Ionophore antibiotics-Valinomycin, Cancer treatment-cisplatin and other Inorganic complexes, Recent Oncology drugs. 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: Enzyme Chemistry

(12 hrs)

Enzymes- Introduction, Metalloenzymes- Zinc enzymes – Carboxy peptidase and Carbonic anhydrase, Iron enzymes – Cytochrome C oxidase, Catalase, Peroxidase and Cytochrome P₄₅₀, Copper enzymes – SOD, Molybdenum oxatransferase enzymes, Xanthine oxidase.

Self-study: Brief study on magnesium enzymes

Unit- V: Selected compounds in Inorganic chemistry

(12 hrs)

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- S₈, S₄²⁺, Se₄²⁺, Te₄²⁺, Squarate, croconate, rhodizionate, Cage compounds-P₄, P₄O₆, P₄O₇, P₄O₈, P₄O₉ and P₄O₁₀, Spinels and Inverse Spinels, Fullerenes, Carbon nanotubes and graphene

Self-study: Molecular materials and fullerides

Text Books:

1. James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Mendhi, Inorganic Chemistry, Principles of Structure and Reactivity, 5th edn., Pearson, 2023.
2. Keith F. Purcell and John C. Kotz, Inorganic Chemistry; Cengage Learning India Pvt. Ltd., New Delhi, 2010.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: New York, 1983.
4. Asim K Das, Bio Inorganic Chemistry.
5. R. Gopalan, V. Ramalingam, Concise Coordination Chemistry, S. Chand, 2001.

Reference Books:

1. Mark Weller, Jonathan Rourke, Tina Overton and Fraser Armstrong, Inorganic Chemistry, Oxford University Press, 6th edn., 2014.

2. Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, Inorganic Chemistry, 5th edn., Oxford University Press, 2010.
3. M.Satake and Y.Mido, Bioinorganic Chemistry- Discovery Publishing House, New Delhi (1996)
4. M.N. Hughes, The Inorganic Chemistry of Biological processes, II Edition, Wiley London, 1982.
5. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
6. R. M. Roat-Malone, Bio Inorganic Chemistry, John Wiley, 2002.
7. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.

MEDICINAL CHEMISTRY

(26PCHE22)

Semester-II

EC-4

Hours/W: 4

Credits: 3

Course Outcomes:

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

CO1: Recall composition and functions of blood, blood groups and Rh factor (K1).

CO2: Explain oxygen transport, anaemia causes and anti-anaemic therapy, lipoprotein metabolism, renal pH regulation and jaundice (K2).

CO3: Apply pharmacological classification to therapeutic use of drugs (K3).

CO4: Compare drug classes (analgesics, antibiotics, anaesthetics, cardiovascular drugs (K4).

CO5: Evaluate clinical test data (LFT, KFT, lipid profile, HbA1c) for diagnosis (K5).

CO6: Integrate biochemical and pharmacological knowledge for patient care (K6).

UNIT-I: Blood, Haematological Agents and Dosage Calculations (12 Hrs)

Composition of blood, Blood grouping and matching, Rh factor, Role of blood as Oxygen carrier, Oxygen cascade, Haematological agents. Anaemia: causes and control. Antianemic drugs. Breakdown of Heme, polycythemia. Methods for calculating drug dosages: Ratio and proportion method, formulation method, dimensional analysis, and Fraction method. Route of administration of drugs.

Self-Study: bombay blood

UNIT-II:

Clinical Chemistry (12 Hrs)

Lipoproteins, Apolipoproteins, Chylomicrons, VLDL, LDL, HDL, Glycated hemoglobin: HbA1C, Liver Function Tests, Kidney Function Tests, Lipid profile, Interpretation of ECG, Renal regulation of pH, Jaundice, Glucose homeostasis and Renin Angiotensin Aldosterone System (RAAS). Pharmacology, Pharmacokinetics and Pharmacodynamics (definitions only) - Drug nomenclature: key suffixes and prefixes to identify drug classes.

Self-Study: HPA axis

UNIT-III: Analgesics, Antibiotics and Anaesthetics (12 Hrs)

Analgesics: Classification of Analgesics-Narcotic analgesics-Non-narcotic analgesics. Antibiotics: Classification of antibiotics, Chloramphenicol, Penicillin, Streptomycin. Anaesthetics: Classification and characteristics of Anaesthetics, Volatile anaesthetics and Non-volatile Anaesthetics, Local Anaesthetics.

Self-Study: Narcotic drugs

UNIT-IV: Bio-Regulatory Drugs**(12 Hrs)**

Cardiovascular drugs - Cardiac glycosides - Anti arrhythmic drugs - Antihypertensive agents Antianginal agents, Diabetes and Hypoglycemic drugs - Types of diabetes, Control of diabetes, Insulin, Oral Hypoglycemic agents - Anti-convulsant agents, Cancer and Antineoplastic drugs, Common Causes, Antimetabolites.

Self-Study: Antiepileptic drugs

UNIT-V: Organic synthesis of some drugs**(12 Hrs)**

Introduction, synthesis and medicinal importance of Thiopental, Diazepam, Captopril, Phenytoin, Salbutamol, Glyburide, Ondansetron, Alprazolam, Thalidomide, Ethambutol, Omeprazole. Paracetamol, Ibuprofen and Ciprofloxacin.

Self-Study: Synthesis of aspirin.

Text Books:

1. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry,
2. Wilson, Beale, John Marlowe; Block, John H, Lipincott William, 12th edition, 2011.
3. Graham L. Patrick, An Introduction to Medicinal Chemistry, 5th edition, Oxford University Press, 2013.
4. Jayashree Ghosh, A text book of Pharmaceutical Chemistry, S. Chand and Co. Ltd, 1999, 1999 edn.
5. D. M. Vasdevan, A Textbook of Biochemistry, Jaypee Brothers Medical Publishers (P) Ltd, 2011, New Delhi.
6. C. C. Chatterjee, Human Physiology, eleventh Coloured Edition, CBS Publishers, 2017, New Delhi.
7. S. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, 1993

Reference Books:

1. Foye's Principles of Medicinal Chemistry, Lipincott Williams, Seventh Edition, 2012
2. Burger's Medicinal Chemistry, Drug Discovery and Development, Donald J. Abraham, David P. Rotella, Alfred Burger, Academic press, 2010.
3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, John M. Beale Jr and John M. Block, Wolters Kluwer, 2011, 12th edn.
4. S. Ramakrishnan, K. G. Prasanna and R. Rajan, Textbook of Medical Biochemistry, Hyderabad: Orient Longman. 3rd edition, 2001.

ANALYTICAL AND GREEN CHEMISTRY

(26PCHS21)

Semester-II

SEC-1

Hours/W: 4

Credits: 2

Course Outcomes:

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

CO1: Recall principles and classification of chromatographic, electroanalytical, spectroanalytical and thermoanalytical techniques (K1).

CO2: Describe thermal decomposition of inorganic hydrates and phase transitions (K2).

CO3: Apply green chemistry principles to reactions and solvent selection (K3).

CO4: Analyze chromatographic separations and electrochemical behavior of species, Interpret TGA, DTA and DSC curves (K4).

CO5: Critically evaluate green catalysts, solvents and synthetic strategies (K5).

CO6: Design green synthetic routes using eco-friendly solvents and catalysts (K6).

UNIT-I: Chromatographic and Thermoanalytical Techniques (12Hr)

Classification of Chromatographic techniques, Partition Chromatography, Paperchromatography, Adsorption chromatography, Column chromatography, Thin-layer chromatography, HPLC. Thermoanalytical techniques: TGA- Principle, Decomposition of Calcium oxalate monohydrate and copper sulphate pentahydrate. Thermal behavior of copper sulphate pentahydrate by DTA. Phase transition studies by DSC- study of glass transition temperature.

Self-Study: Chiral chromatography and enantiomeric separations.

UNIT-II: Electroanalytical and Spectro Analytical Techniques (12 Hr)

Electroanalytical techniques – Principle, Instrumentation (Block diagram) and applications. Electrogravimetry, Electrolytic separation and estimation of metal ions. Coulometry: Coulometric titrations, separation of nickel and cobalt, amperometry, cyclic voltammetry, principle and applications. Spectro-analytical methods – principle and applications of Colorimetry, Spectrophotometry, Nephelometry, Turbidimetry, Atomic absorption spectroscopy.

Self-Study: AI-assisted spectral interpretation.

UNIT- III: Introduction to Green Chemistry (12 Hr)

Introduction- Need for Green Chemistry. Goals of Green Chemistry. Twelve principles of Green Chemistry with examples. Concept of atom economy. Micro wave assisted reactions: Introduction Principle. Microwave assisted reactions in water: Hofmann elimination, Oxidation of toluene. Microwave assisted solvent free reactions: Deprotection, synthesis of pyridines.

Self-Study: E-factor, Process Mass Intensity (PMI), Carbon Efficiency.

UNIT – IV: Green Solvents and Green Synthesis (12 Hr)

Green solvents: Supercritical carbon dioxide, Ionic liquids, Water, Organic synthesis in solid state. Designing a green synthesis: Choice of starting materials, Choice of reagents, Choice of catalysts and Choice of solvents. Green synthesis-adipic acid, BHT and catechol. Green chemistry in day today life.

Self-Study: Switchable solvents.

UNIT– V: Green Catalysts (12 Hr)

Phase transfer catalysis in green synthesis: Mechanism, types of PTC. Applications: Nitriles from alkyl halides, Alcohols from Alkyl halides. Organic synthesis using crown ethers: esterification, saponification, anhydride formation, Elimination reaction, Displacement reaction. Ultrasound assisted reactions: Coupling reactions, Cannizaro reaction. Self-Study: Chiral phase transfer catalysts.

Text Books:

1. V. Kumar, An introduction to green chemistry, Vishal publishing Co, 2007, New Delhi.
2. V. K. Ahluwalia, A text book of Green Chemistry, Narosa Publishing House Pvt Ltd, 2013, New Delhi.

Reference Books:

1. Indu Tucker Sidhwani and Rakesh K. Sharma, An introductory textbook of Green chemistry, Wiley publications, 2020, New Delhi.
2. Anju Srivastava and Rakesh K Sharma, Green Chemistry for Beginners, 2021 by Jenny Stanford Publishing, New Delhi.

ORGANIC CHEMISTRY-III
(26PCHC31)

Semester-III

Core-09

Hours/W: 5

Credits: 5

Course Outcomes:

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

CO1: Recall principles and instrumentation of UV-Vis, IR, ^1H NMR, ^{13}C NMR and Mass spectroscopy (K1).

CO2: Describe NMR chemical shift, coupling, NOE and spectral simplification methods (K2).

CO3: Explain mass spectral peaks, isotopic patterns and fragmentation mechanisms (K3).

CO4: Apply Woodward-Fieser and IR correlation rules to predict spectral features (K4).

CO5: Evaluate competing mechanisms in addition and rearrangement reactions (K5).

CO6: Design synthetic routes employing addition, name and rearrangement reactions (K6).

UNIT-I: UV and IR SPECTROSCOPY

(15 Hrs)

UV-VIS Spectroscopy: Basic principle – the absorption laws – types of electronic transitions- effects influence of solvent and H-bonding on λ_{max} values. Woodward-Fischer rules to calculate λ_{max} values of conjugated dienes and α , β – unsaturated ketones and Scott's rule. Infra-Red Spectroscopy (IR): Basic principle – Types of Molecular Vibrations in IR Spectroscopy, Characteristic of IR absorptions of different functional groups—factors influencing the IR absorption of molecules of carbonyl group: electronic effect, hydrogen bonding and Fermi resonance.

Self-Study: Solvatochromism and bathochromic/hypsochromic shifts.

UNIT-II: ^1H NMR and ^{13}C NMR SPECTROSCOPY

(15 Hrs)

^1H - NMR spectroscopy: Basic principle- Number of signals- Chemical shift-shielding and deshielding -Factors influencing the chemical shifts - Spin-spin coupling - Coupling constant and factors influencing the coupling constant -Simplification of spectra: Lanthanide Shift reagents, deuterium exchange reaction, NOE effect and spin decoupling. ^{13}C -NMR spectroscopy - Basic principle- 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). Introduction to 2D NMR - COSY, NOESY.

Self-Study: DEPT-45, DEPT-90, and DEPT-135 experiments.

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, Retro Diels-Alder reaction, ortho effect - Fragmentation pattern of simple compounds of amines, ketones, acids and phenols.

Self-Study: Electrospray Ionization (ESI).

UNIT-IV: ORGANIC REACTION MECHANISM

(15 Hrs)

Orientation and reactivity, hydrogenation of double and triple bonds, Michael reaction, Addition to carbon-hetero atom multiple bonds: Mannich reaction, acids, esters, nitrites, addition of Grignard reagents, Wittig reaction, Prins reaction, Stobbe reactions. Name reactions: Jones Oxidation, Dakin reaction, Mukaiyama reaction, Pechmann Condensation, Suzuki and Mitsunobu reaction. von Richter, Sommelet- Hauser and Smiles rearrangements.

Self-Study: Heck and Sonogashira coupling reactions.

UNIT-V: REARRANGEMENTS AND APPLICATIONS

(15 Hrs)

Rearrangements to electron deficient carbon: Pinacol-pinacolone and semi-pinacolone rearrangements and applications. Wagner-Meerwein, Demjanov, Baker-Venkataraman, Benzilic acid and Wolff rearrangements. Rearrangements to electron deficient nitrogen: Hofmann, Curtius, Schmidt, Lossen and Beckmann rearrangements. Rearrangements to electron deficient oxygen: Baeyer-Villiger oxidation. Rearrangements to electron rich atom: Favorskii, Stevens, [1,2]-Wittig and [2,3]-Wittig rearrangements. Fries and Photo Fries rearrangement. Intramolecular rearrangements – Claisen, Cope, oxy-Cope rearrangements.

Self-Study: Enzymatic Baeyer–Villiger oxidation.

Text Books:

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.
3. P.De Mayo, ‘Molecular Rearrangements’
4. Jerry March, “Advanced Organic Chemistry”, Student Wiley 4th edition, Reprint 2003
5. I.L. Finar, Organic Chemistry, Vol. I &II, 3rd Indian Reprint, 2001, Pearson Education,.
6. R.O.C. Norman, Organic Synthesis, 2nd ed.

Reference Books:

1. Donald L. Pavia, Gary M. Lampman, George A. Kriz and James R. Vyvyan.

- Introduction to Spectroscopy, Cengage India Private Limited, 2015, Noida
2. P S Kalsi, Spectroscopy of Organic Compounds, New Age International Pvt Ltd, 2024, Daryaganj New Delhi
 3. P S Kalsi, Spectroscopy of Organic Compounds, New Age International Private Limited, 2020, Daryaganj, NewDelhi.

INORGANIC CHEMISTRY – II

(26PCHC32)

Semester-III

Core-10

Hours/W: 5

Credits: 5

Course Outcomes:

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

CO1: Recall electronic configurations, periodic trends, coordination theories, reaction types, silicate classifications, metal carbonyls, photochemical laws, structures of boranes and metal clusters (K1)

CO2: Explain variable valency, magnetic and spectral properties, lanthanide contraction, CFSE, Jahn–Teller effect, trans effect, substitution and electron transfer mechanisms, multi-centered bonding, Wade–Mingos rules, and principles of inorganic photochemistry. (K2)

CO3 : Apply CFT, MOT, kinetic theories, and bonding rules (Wade, Lipscomb, Jemmis mno rule) to predict structure, stability, reactivity, and magnetic behaviour of coordination compounds, boranes, silicates, and metal clusters. (K3)

CO4: Analyze mechanisms of substitution and electron transfer reactions, interpret spectroscopic and magnetic data, evaluate photo-induced processes, and differentiate structural types of inorganic chains, rings, cages, and clusters. (K4)

CO5: Evaluate stability trends across transition and inner transition elements, assess theoretical limitations (VB, CFT), compare lanthanides and actinides, and critically examine catalytic, photochemical, and structural behaviour of advanced inorganic systems. (K5)

CO6: Design mechanistic pathways, predict structures of novel coordination compounds and clusters(K6)

Unit-I Transition Elements and Inner transition Elements

15hrs

Transition elements- Electronic structure - General characteristics - atomic, ionic radii – variation along the period and group. Variable valency, colour, magnetic properties, non-stoichiometric, catalytic property and complexing tendency- Comparison of first row with other two rows of transition elements. Stabilization of unusual oxidation states. Inner transition elements - position in the periodic table – electronic configuration, oxidation states, colour and spectra, magnetic properties. Separation of lanthanides –Valency change and Ion exchange method. Lanthanide contraction- Cause and consequences, 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 using photoelectron 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- Outer-sphere mechanisms and Inner-sphere mechanisms. Complementary, non-complementary reactions.

Self-study: Stereochemistry and isomerization of complexes

Unit- IV: Inorganic chains, rings, cages**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 $[\text{TeMo}_6\text{O}_{24}]^{6-}$ and $[\text{Mo}_7\text{O}_{24}]^{6-}$ 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_6H_{10} , B_8H_{12} , $\text{B}_{10}\text{H}_{14}$, $\text{B}_{12}\text{H}_{12}^{2-}$ STYX code-Lipscomb rule. Wade and Mingo's rule to identify types of boranes and carboranes. Low and High nuclearity metal carbonyls.

Self-study: Jemmis mno rule

Unit-V: Inorganic photochemistry and Metal Clusters**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 Ru polypyridyl complexes. Photochemical conversion and storage of solar energy-ruthenium complex

Metal clusters- dinuclear cluster- $\text{Re}_2\text{Cl}_8^{2-}$ and dinuclear Re and Mo analogues, trinuclear cluster- Re_3Cl_9 , tetranuclear clusters- $\text{W}_4(\text{OR})_{16}$, hexanuclear clusters- $\text{M}_6\text{Cl}_{12}^{2+}$, $\text{M}_6\text{Br}_8^{4+}$ - Mo, W, Nb and Ta. Polyatomic Zintl anions and cations.

Self-study: Chevrel phases

Text Books:

1. J. D. Lee, Concise Inorganic Chemistry, Blackwell Science, 5th edn., 2011.
2. J E Huheey, EA Keiter, RL Keiter and OK Medhi, Inorganic Chemistry – Principles of structure and reactivity, 4th Edition, Pearson Education Inc., 2006
3. G L Meissler and D ATarr, Inorganic Chemistry, 3rd Edition, Pearson Education Inc., 2008,
4. D. Bannerjea, Co-ordination Chemistry, TATA Mcgraw Hill, 1993.
5. B. N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd, 1976.
6. F. A. Cotton, G. Wilkinson.; C. A. Murillo; M. Bochmann, Advanced Inorganic Chemistry, 6th ed.; Wiley Inter-science: New York, 1988

Reference Books:

1. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, Saunders Publications, USA, 1977.
2. Peter Atkins and Tina Overton, Shriver and Atkins' Inorganic Chemistry, 5th Edition, Oxford University Press, 2010.
3. Mandeep Dalal, A Text book of Inorganic chemistry, vol.1, International edition, 1st edn., 2012.
4. Basic Inorganic Chemistry, F. A. Cotton, G. Wilkinson, P. L. Gauss, John Wiley, 2002, 3rd edn.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edn, John Wiley, 1994,.
6. D. F. Shriver, P. W. Atkins, Inorganic Chemistry, W. H. Freeman and Co, London, 2010.

PHYSICAL CHEMISTRY-II

(26PCHC33)

Semester-III

CORE-11

Hours/W: 5

Credits:5

Course Outcomes:

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

CO1: Explain the classical and statistical concepts of thermodynamics(K1).

CO2: Discuss the various thermodynamic and kinetic determination (K2).

CO3: Compute the theories of reaction rates and fast reactions (K3).

CO4: Correlate the thermodynamic concepts to study the kinetics of chemical reactions (K4).

CO5: Evaluate the thermodynamic methods for real gases and mixtures(K5).

CO6: Integrate the classical and statistical thermodynamics(K6).

UNIT-I: Classical Thermodynamics

(15 Hrs)

Partial molar properties-Chemical potential, Gibb's- Duhem equation-binary and ternary systems. Determination of partial molar quantities. Thermodynamics of real gases - Fugacity- determination of fugacity by graphical and equation of state methods-dependence of temperature, pressure and composition. Thermodynamics of ideal and non-ideal binary mixtures, Duhem -Margulis equation applications of ideal and non-ideal mixtures. Activity and activity coefficients-standard states.

Self-Study: van der Waals, Redlich-Kwong, Soave-Redlich-Kwong, and Peng-Robinson equations.

UNIT-II: Statistical thermodynamics

(15 Hrs)

Introduction of statistical thermodynamics concepts of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics- comparison and applications. Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions-calculation of equilibrium constants. Statistical approach to Thermodynamic properties: pressure, internal energy, entropy, enthalpy, Gibb's function, Helmholtz function, equilibrium constants and equipartition principle. Heat capacity of solids-Einstein and Debye models.

Self-Study: Monte Carlo methods.

UNIT-III: Irreversible Thermodynamics**(15 Hrs)**

Theories of conservation of mass and energy entropy production in open systems by heat, matter and current flow, force and flux concepts. Onsager theory-validity and verification- Onsager reciprocal relationships. Electro kinetic and thermomechanical effects- Application of irreversible thermodynamics to biological systems.

Self-Study: Onsager–Casimir reciprocal relations.

UNIT-IV: Chemical Kinetics-I**(15 Hrs)**

Theories of reactions-effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis-molecular beams, collision cross sections, effectiveness of collisions,Potential energy surfaces. Transition state theory-evaluation of thermodynamic parameters of activation-applications of ARRT to reactions between atoms and molecules, Factors determine the reaction rates in solution - primary salt effect and secondary salt effect, Homogeneous catalysis- acid- base catalysis-mechanism of acid base catalysed reactions-Bronsted catalysis law, enzyme catalysis-Michaelis-Menton catalysis.

Self-Study: Allosteric enzymes.

UNIT-V: Chemical Kinetics-II**(15 Hrs)**

Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. Chain reactions-chain length, kinetics of $\text{H}_2 - \text{Cl}_2$ & $\text{H}_2 - \text{Br}_2$ reactions (Thermal and Photochemical reactions) - Rice Herzfeld mechanism(Pyrolysis of acetaldehyde). Study of fast reactions-relaxation methods- temperature and pressure jump methods electric and magnetic field jump methods -stopped flow flash photolysis methods and pulse radiolysis.

Self-Study: Atmospheric free-radical chemistry.

Text Books:

1. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd edition,S.L.N.Chand and Co., Jalandhar, 1986.
2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A. BenjaminPublishers, California, 1972.
3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995.
4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013.

Reference Books:

1. D.A. Mcquarrie and J.D.Simon, Physical Chemistry - A Molecular Approach, Viva Books Pvt. Ltd., NewDelhi, 1999.
2. R.P. Rastogi and R.R.Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi,1990.
3. S.H. Maron and J.B.Lando, Fundamentals of Physical Chemistry, Macmillan Publishers, New York, 1974
4. K.B. Ytsimiriski, "Kinetic Methods of Analysis", Pergamom Press,1996.

PHYSICAL CHEMISTRY PRACTICAL-I

(26PCHC34)

Semester-III

Core-12

Hours/W: 5

Credits: 2

Course Outcomes:

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

CO1: summarize the principles of conductometry, thermochemistry and potentiometry (K2)

CO2: perform the conductometric titrations between acids and salt mixtures against bases and apply the electrochemical methods for determining its concentration. (K3)

CO3: determine the pK_a and K_a values of the weak acid by titrating against a strong base using a quinhydrone electrode. (K4) record and interpret the experimental data and construct acid- base graph (K4)

CO4: Prepare different buffer solutions and can determine the pH values of buffer solutions and solubility products by using quinhydrone electrode and glass electrode. (K5)

CO5: justify the validity of Debye-Huckel Onsager theory (K5)

UNIT-I: Conductivity Experiments

1. Determination of equivalent conductance of a strong electrolyte & the verification of DHO equation.
2. Verification of Ostwald's Dilution Law & Determination of pK_a of a weak acid.
3. Verification of Kohlrausch's Law for weak electrolytes.
4. Determination of solubility of a sparingly soluble salt.
5. Acid-base titration (strong acid and weak acid vs NaOH).
6. Precipitation titrations (mixture of halides only).
7. Determination of strength of sodium acetate and acetic acid in an acetic buffer

UNIT-II: Potentiometric Experiments

1. Acid-Base titrations (SA and WA vs NaOH)
2. Dissociation constant of acetic acid in dioxane and water by titrating with KOH
3. Solubility product of AgX
4. Estimation of halides in water samples by potentiometry

Text Books:

1. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.

2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.
3. V.D. Athawale and Parul Mathur, Experimental Physical Chemistry, New Age International (P) Ltd., New Delhi, 2008.
4. E.G. Lewers, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Ed., Springer, New York, 2011.

References:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.
4. Shailendra K Sinha, Physical Chemistry: A laboratory Manual, Narosa Publishing House Pvt, Ltd., New Delhi, 2014.
5. F. Jensen, Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell.

ANALYTICAL INSTRUMENTATION TECHNIQUES

PRACTICALS

(26PCHC35)

Semester-III

CORE-13

Hours/W: 4

Credits: 2

Course Outcomes:

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

CO1: understand the principles associated with various inorganic organic and physical chemistry experiments (K2).

CO2: analyse different constituents through instrumental methods of analysis (K4).

CO3: evaluate different contaminants in materials using turbidimetry and conductivity measurements (K5).

CO4: design chromatographic methods for identification of species (K6).

UNIT-I Chromatographic Analysis and Instrumental Analysis

1. Paper Chromatography-

- a) Separation of dyes
- b) Separation of mixture of metal ions

2. Thin Layer Chromatography-

- a) Separation of mixture of organic compounds (two component)
- b) Purity check of p-nitroacetanilide
- c) Check the purity of analgesic drug

3. Column Chromatography

- a) Separation of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$
- b) Plant pigments separation by using column chromatography

4. Study of Tanabe-Sugano diagram of metal complexes by UV-VIS spectroscopy.

5. Simultaneous estimation of Mn and Cr from an unknown mixture by spectrophotometer.

6. Estimation of Ca, Pb, and Zn by AAS.

UNIT-II: Interpretation and identification of the given spectra of various organic compounds arrived at from the following instruments

- 1. UV-Visible
- 2. IR
- 3. Raman
- 4. NMR
- 5. ESR
- 6. Mass

Text Books:

1. Vogel's Text book of Practical Organic Chemistry, 5th Ed, ELBS/Longman, England, 2003.
2. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis; 6th ed., ELBS, 1989.
3. J. D. Woollins, Inorganic Experiments; VCH: Weinheim, 1995.
4. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.
5. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S.Viswanathan Co. Pvt., 1996.

Reference Books:

1. N. S. Gnanapragasam and G. Ramamurthy, Organic Chemistry – Labmanual, S. Viswanathan Co. Pvt. Ltd, 2009.
2. J. N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 2011.
3. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
4. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
5. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.

BIOMOLECULES AND HETEROCYCLIC COMPOUNDS

(26PCHE31)

Semester-III

EC-5

Hours/W: 4

Credits: 3

Course Outcomes:

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

CO1: learn the basic concepts and biological importance of biomolecules and natural products (K1).

CO2: explain various of functions of carbohydrates, proteins, nucleic acids, steroids and hormones (K2).

CO3: integrate and assess the different methods of preparation of structurally different biomolecules and natural products (K3).

CO4: illustrate the applications of biomolecules and their functions in the metabolism of living organisms (K4).

CO5: analyse and rationalise the structure and synthesis of heterocyclic compounds (K5).

CO6: develop the structure of biologically important heterocyclic compounds by different methods (K6).

UNIT-I: Chemistry of carbohydrates

(12 Hrs)

Definition, classification and biological role of carbohydrates. monosaccharides:

Linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose (structure determination not required), Disaccharides: Ring structures (Haworth formula) of Polysaccharides: Starch, glycogen and cellulose (structure only).

Self-Study: O-, N-, and S-glycosides.

UNIT-II: Steroids and Hormones

(12 Hrs)

Steroids-Introduction, occurrence, nomenclature, configuration of substituents. Diels' hydrocarbon, stereochemistry, classification, biological importance of cholesterol. Hormones-Introduction, classification, functions of sex hormones- androgens and estrogens, adrenocortical hormones-cortisone and cortisol structure and functions of non-steroidal hormones-adrenaline and thyroxin.

Self-Study: Vitamin D role in calcium metabolism

UNIT-III: Proteins and nucleic acids

(12 Hrs)

Separation and purification of proteins – dialysis, gel filtration and electrophoresis. Catabolism of amino acids – transamination, oxidative deamination and decarboxylation. Structure, methods for the synthesis of nucleosides – direct combination, conversion of

nucleoside to nucleotides. Primary and secondary structure of RNA and DNA, Watson-Crick model.

Self-Study: Protein Sequencing Methods-Edman degradation.

UNIT-IV: Amino acids and Vitamins (12 Hrs)

Introduction, classification, stereochemistry of amino acids, separation. Vitamins- Definition, classification, structure, synthesis and functions of Vitamins A, D, E, K, C and B (Structural elucidation is not required)

Self-Study: Oxidative stress and free-radical protection.

UNIT-V: Fused Ring Heterocyclic Compounds (12 Hrs)

Benzo fused five membered rings: Indole, isoindole and benzofuran. Preparation and properties. Benzo fused six membered rings: Quinoline and isoquinoline: Preparation by ring closure reactions, Reactions: Electrophilic and nucleophilic substitutions, oxidation and reduction reactions. (Mechanism not required).

Self-Study: Medicinal Importance of Fused Heterocycles

Text Books:

1. T. K Lindhorst, Essentials of Carbohydrate Chemistry and Biochemistry, Wiley VCH, North America, 2007.
2. I. L. Finar, Organic Chemistry Vol-2, 5th edition, Pearson Education Asia, 1975.
3. V. K. Ahluwalia and M. Goyal, Textbook of Heterocyclic compounds, Narosa Publishing, New Delhi, 2000.
4. M. K. Jain and S. C. Sharma, Modern Organic Chemistry, Vishal Publishing Co., Jalandhar, Delhi, 2014.
5. V. K. Ahluwalia, Steroids and Hormones, Ane books pub., New Delhi, 2009.

Reference Books:

1. I. L. Finar, Organic Chemistry Vol-1, 6th edition, Pearson Education Asia, 2004.
2. Pelletier, Chemistry of Alkaloids, Van Nostrand Reinhold Co, 2000.
3. Shoppe, Chemistry of the steroids, Butterworths, 1994.
4. I. A. Khan, and A. Khanum. Role of Biotechnology in medicinal & aromatic plants, Vol 1 and Vol 10, Ukkaz Publications, Hyderabad, 2004.
5. M. P. Singh. and H. Panda, Medicinal Herbs with their formulations, Daya Publishing House, Delhi, 2005.

**RESEARCH METHODOLOGY AND CHEMINFORMATICS
(26PCHS31)**

Semester-III

SEC-2

Hours/W: 3

Credits: 2

Course Outcomes:

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

CO1: Recall primary and secondary chemical literature sources, databases and citation indexes (K1)

CO2: Explain principles of molecular modelling, DFT and spectral prediction (K2)

CO3: Apply chemoinformatics tools for property and activity prediction (K3)

CO4: Analyze structure–property and structure–spectra correlations (K4)

CO5: Critically assess ligand-based and structure-based drug design methods (K5)

CO6: Propose computer-assisted synthesis or structure elucidation strategies (K6)

Unit-I: Literature survey (9 Hr)

Journals, patents, reviews, monographs, text books and Journal Impact factor. Literature searching-science citation index and locating journals (articles), information retrievals with internet. Research paper format in Indian journal Chemistry, Indian Journal of Chemical Society, Journal of American Chemical Society, RSC, Wiley, Springer link and Tetrahedron. In-depth study of two papers from any leading international journals.

Self-Study: h-index, i10-index, g-index, and other research metrics

UNIT II: Chemdraw and Gaussian (9 Hr)

Chemdraw basics: Starting Chemdraw, predicting the IUPAC name from the structure and vice versa. Gaussian: Drawing the chemical structure in the Gaussview, optimization, DFT calculation: UV, IR and ¹H and ¹³C NMR theoretical spectral prediction. HOMO–LUMO calculations.

Self-Study: Electronegativity calculations

Unit -III: Computer in Research

Excel: Manage rows/columns in table, Shortcuts in Excel. Core Math Functions: Master SUM, AVERAGE, COUNT, MIN, and MAX. Build and customize Pivot Tables.

Origin: Importing data, adding data, managing column designations, generating line, scatter, statistical, and contour plots. Creating, customizing, and formatting 2D and 3D.

Self-Study: Interconversion of chemical file formats.

Unit-IV: Introduction to Cheminformatics: (9 Hr)

Tools used in cheminformatics. Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations,

Structure of Molfiles and Sdfiles, Libraries and toolkits. Full structure search, sub-structure search, similarity search, three dimensional search methods.

Self-Study: Chemical Data Mining

UNIT V: Applications

(9 Hr)

Computer-Assisted Synthesis Design, Introduction to Drug Design, Target Identification and Validation, Lead Finding and Optimization, Analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-Based and Structure-Based Drug Design.

Self-Study: ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) modeling.

Text Books:

1. Andrew R. Leach & Valerie, J. Gillet (2007). An introduction to Chemoinformatics. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003). Chemoinformatics: A text-book. Wiley-VCH.

Reference Book:

1. Gupta, S. P. (2011). QSAR & Molecular Modeling. New Delhi: Anamaya Pub.

INTERNSHIP
(23PCHI35)

Semester-III

Internship

Credits: 2

- Carried out in summer vacation at the end of second semester.
- Report submission.

INORGANIC CHEMISTRY – III

(26PCHC41)

Semester-IV

CORE-14

Hours/W: 6

Credits: 5

Course Outcomes:

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

CO1: Recall and define fundamental concepts of organometallic compounds, bioinorganic systems, catalytic processes and spectroscopic techniques including structure, bonding, nomenclature, and key industrial processes. (K1)

CO2: Explain the structure, bonding, stability and reactivity of organometallic complexes using EAN rule, 18-electron rule, ligand field theory, and spectroscopic principles (K2)

CO3: Apply electron counting methods, reaction mechanisms and spectroscopic techniques to interpret structures, predict stability and analyze experimental data of inorganic and organometallic systems. (K3)

CO4: Analyze reaction mechanisms, catalytic pathways, electronic transitions and bioinorganic processes by correlating theoretical concepts with structural and spectroscopic evidence. (K4)

CO5: evaluate the efficiency and mechanistic aspects of homogeneous and heterogeneous catalysis, metalloprotein function, and spectroscopic methods for structural elucidation. (K5)

CO6: Design mechanistic pathways, propose catalytic cycles, and construct structural interpretations for unknown organometallic and bioinorganic systems using combined spectroscopic and theoretical approaches. (K6)

Unit- I: Organometallic chemistry-I

(18 hrs)

Metal carbonyls - Structures of $\text{Fe}(\text{CO})_5$, $\text{Fe}_2(\text{CO})_9$, $\text{Fe}_3(\text{CO})_{12}$, $\text{Co}_2(\text{CO})_8$, $\text{Mn}_2(\text{CO})_{10}$, $\text{Os}_4(\text{CO})_{14}$ – 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 of metal carbonyls and main group fragments

Unit- II: Organometallic Chemistry - II**(18 hrs)**

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

Self-study: Electro catalysis and photo catalysis

Unit- IV: Physical methods in Inorganic chemistry – I**(18 hrs)**

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. Photoelectronic spectra of N_2 , O_2 , CO and H_2O molecules.

Self-study: Magnetism of complexes

Unit- IV: Physical methods in Inorganic chemistry II**(18 hrs)**

Nuclear magnetic resonance (NMR). Applications of multiprobe NMR to inorganic compounds- ^{31}P -NMR spectra of P_4S_3 , H_3PO_3 , H_3PO_2 , HPF_2 , $\text{HP}_2\text{O}_5^{3-}$ ^{19}F -NMR spectra of ClF_3 and BrF_3 . ^{11}B NMR spectrum of $\text{B}_{10}\text{H}_{14}$. 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: Bio-Inorganic Chemistry-I**(18 hrs)**

Metalloporphyrins- The interaction between heme and dioxygen, cyanide and carbon monoxide poisoning. Myoglobin and Hemoglobin- Bohr effect, Hill constant and cooperativity effect. Hemerythrin and Hemocyanin. Cytochromes, Iron-sulphur proteins- Rubredoxin and Ferredoxin, Blue Copper proteins. Chlorophyll- structure and function. Photo synthetic electron transport sequence, Vitamin- B_{12} and B_{12} Coenzymes. Nitrogen fixation – *In-vitro* and *in-vivo* nitrogen fixation.

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

Text Books:

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, 6th 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

Reference Books:

1. Mark Weller, Tina Overton, Jonathan Rourke and Fraser Armstrong, Inorganic chemistry, 6th edition, Oxford University Press, 2014.
2. D.Sutton – Electronic spectroscopy of transition metal complexes, McGraw – Hill.
3. Lippard, Berg, Bertini and Valentine, Bio- inorganic chemistry, University Science Books.
4. AsimK.Das, Bioinorganic chemistry, Books and Allied (p) Ltd.
5. R.Gopalan and V. Ramalingam – Concise coordination chemistry, University Science Books.

PHYSICAL CHEMISTRY-III

(26PCHC42)

Semester-IV

Core-15

Hours/W: 6

Credits: 5

Course Outcomes:

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

CO1: knowledge on storage devices and electrochemical reaction mechanism (K1).

CO2: understand the behaviour of electrolytes in solution and compare the structures of electrical double layer of different models (K2).

CO3: highlight the different types of over voltages and its applications in electroanalytical techniques (K3).

CO4: discuss the theories of electrolytes, electrical double layer, electrodictics and activity coefficient of electrolytes (K4).

CO5: discuss the mechanism of electrochemical reaction and different thermodynamic mechanism of corrosion (K5).

CO6: predict the kinetics of electrode reactions applying Butler-Volmer and Tafel equations. (K6).

UNIT-I: Electrochemistry-I (Ionics)

(18 Hrs)

Fundamentals of electrochemistry – Electrochemical cells-two and three electrode system Electrochemistry of solutions containing ions: influence of temperature and pressure on ionic conductance – 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) - The Huckel and Bronsted equations.

Self-Study: Evidence for ionic atmosphere.

UNIT-II: Electrode-electrolyte interface and Elementary Electrodic Reactions

(18 Hrs)

Significance of electrode-electrolyte interface between conducting phases- formation of electrical double layer (EDL)- contributions to the total potential difference- concept of surface excess- electrocapillarity, electrocapillary curves, Lippmann equation of electrocapillarity (Derivation not required). 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- Tafel equation and Tafel plot.

Self-study: Bjerrum model

UNIT-III: Electrodicts of Multistep Multi Electron System (18 Hrs)

Rates of multi-step electrode reactions, Butler - Volmer equation for a multi-step reaction. Rate determining step, electrode polarization and depolarization. Transfer coefficients, its significance and determination, Stoichiometric number. Electro-chemical reaction mechanisms-rate expressions, order, and surface coverage.

Electrokinetic phenomena: Electroosmosis and electrophoresis- determination of zeta potentials Departure from equilibrium- kinetics of hydrogen evolution-theories of hydrogen overvoltage- oxygen overvoltage – over potential and polarization.

Self-Study: Electrocatalysts for hydrogen production.

UNIT-IV: Polymer Chemistry (18 Hrs)

Overview and Classification of Polymers – Kinetics of polymerization: Kinetics of addition polymerization, kinetics of condensation polymerization. Kinetics of Free radical chain polymerization. Determination of molar masses of polymers by osmotic pressure method and viscometry. Number-average molecular weight and Weight-average molecular weight. Vulcanization of rubber, plasticizers. Structure of crystalline and amorphous polymers, Glass transition temperature (T_g) – factors influencing the T_g. Electronically conducting polymers: Poly(Sulphur Nitride), Poly(para-phenylene). Fire-retardant polymers.

Self-Study: Flory-Huggins Theory

UNIT-V: Surface Chemistry and Colloids (18 Hrs)

Types of adsorption and isotherm, Langmuir, Freundlich, B.E.T and Gibb's adsorption isotherm, calculation of surface area of solids. concept of positive and negative adsorption, Langmuir-Hinshelwood and Eley-Rideal mechanisms.

Lyophilic, lyophobic, and association colloids. Origin of surface charge: Helmholtz-Perrin, Gouy-Chapman, and Stern models. Coagulation of colloidal sols and Schulze-Hardy rule. Surfactants and classification, micelle formation, Critical Micelle Concentration (CMC), Kraft point. Emulsification by surfactants.

Self-Study: HLB value

Text Books:

1. D. R. Crow, Principles and applications of electrochemistry, 4th edition, Chapman & Hall/CRC, 2014.
2. J. Rajaram and J.C. Kuriakose, Kinetics and Mechanism of chemical transformations Macmillan India Ltd., New Delhi, 2011.
3. S. Glasstone, Electro chemistry, Affiliated East-West Press, Pvt., Ltd., New Delhi, 2008.

Reference Books:

1. J.O.M. Bockris and A.K.N. Reddy, Modern Electro chemistry, vol.1 and 2B, Springer, Plenum Press, New York, 2008.
2. J.O.M. Bockris, A.K.N. Reddy and M.G. Aldeco Morden Electro chemistry, vol. 2A, Springer, Plenum Press, New York, 2008.
3. Philip H. Rieger, Electrochemistry, 2nd edition, Springer, New York, 2010.
4. L.I. Antropov, Theoretical electrochemistry, Mir Publishers, 1977.
5. K.L. Kapoor, A Text book of Physical chemistry, volume-3, Macmillan, 2001.

PROJECT WITH VIVA VOCE

(26PCHC43)

Semester-IV

Core-16

Hours/W: 10

Credits: 7

Structure of the Project Report

1. Cover Page
2. Certificate
3. Declaration
4. Acknowledgement
5. Chapter-I Introduction
6. Chapter-II
7. Chapter-III
8. Chapter-IV
9. Chapter-V Conclusion and Scope for further research Assessment

Internal: 100 Marks

External: 100 Marks

PHYSICAL CHEMISTRY PRACTICAL-II

(26PCHE41)

Semester-IV

EC-6

Hours/W: 4

Credits: 3

Course Outcomes:

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

CO2: determine the kinetics of adsorption of oxalic acid on charcoal (K3).

CO3: evaluate the order of the reaction, temperature coefficient, and activation energy of the reaction by following pseudo first order kinetics. (K5).

CO4: construct the phase diagram of two component system forming congruent melting solid and find its eutectic temperatures and compositions. (K6).

CO4: develop the potential energy diagram of hydrogen ion, charge density distribution and Maxwell's speed distribution by computational calculation (K6).

UNIT-I: Kinetics

1. Study the kinetics of acid hydrolysis of an ester, determine the temperature coefficient and also the activation energy of the reaction.
2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half-life method and determine the order with respect to iodine and acetone.
3. Determination of Association factor, distribution constant, association constant and mass of benzoic acid distributed between carbon tetrachloride and water.
4. Determination of rate constant of the redox reaction between KI and K₂S₂O₈. Verification of Bronsted Bjerrum Equation

UNIT-II: Phase diagram

Construction of phase diagram for a simple systems

1. Chloroform- Acetic acid-Water
2. Naphthalene-phenanthrene
3. Benzophenone- diphenyl amine

Unit-III: Adsorption Studies

Adsorption of oxalic acid on charcoal & determination of surface area (Freundlich isotherm only).

Text Books:

1. B. Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009.

2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.
3. V.D. Athawale and Parul Mathur, Experimental Physical Chemistry, New Age International (P) Ltd., New Delhi, 2008.
4. E.G. Lewers, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Ed., Springer, New York, 2011.
5. K. Karunakaran, Laboratory Manuel for Physical Chemistry Practicals.

References:

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J. N. Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.
4. Shailendra K Sinha, Physical Chemistry: A laboratory Manual, Narosa Publishing House Pvt, Ltd., New Delhi, 2014.
5. F. Jensen, Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell.

TRAINING FOR COMPETITIVE EXAMINATION

(26PCHS41)

Semester-IV

SEC-4

Hours/W: 4

Credits: 2

1. Chemistry for UGC-CSIR NET / SET/TRB (2 hours)
2. General studies for UPSC/TNPSC/ other competitive examinations (2 hours)

EXTRA CREDIT COURSES
CHEMISTRY IN CONSUMER PRODUCTS
(26PCHEC1)

Semester-I

ECC-1

Credits: 3

Course Outcomes:

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

CO1: learn about basic knowledge in chemical consumer Products (K1).

CO2: understand the chemical composition and their applications of consumer products (K2).

CO3: make use of applications of milk and milk products(K3).

CO4: classify the soaps, detergents, pigments, perfumes and milk products (K4).

CO5: criticize the bio role and side effects of drugs (K5).

CO6: makeup the day to day life articles(K6).

UNIT-I: SOAPS AND DETERGENTS

Soap — definition and types — manufacture of different types of soaps (toilet soaps, transparent soaps and liquid soaps) and their uses — cleansing action of soaps. Detergents — classification of detergents (cationic, anionic and non-ionic) — comparison of soaps and detergents. Dry cleaning and its effect on the environment.

UNIT- II: PIGMENTS AND PERFUMES

Pigments — Definition — Examples — colours imparted by the pigments and their uses (lithopone, titanium dioxide, ultramarine blue, Red lead, chrome green). Perfumes — Ingredients of perfumes- Isolation of essential oils — Artificial flavours — apple, grape, banana, pineapple, jackfruit (Naming of a few compounds only structure not needed)

UNIT -III: DRUGS CHEMISTRY

Drugs- Definition — Importance of some common drugs with examples — mouth washes — antacids — analgesics — antipyretics — sedatives and hypnotics. Anaesthetics — Basic requirements of anaesthetics — Classification with examples — distinction between antiseptics and disinfectants.

UNIT-IV: CHEMISTRY OF FIREWORKS

Gun powder-process of making Cobra eggs magic serpent, manufacture of toy caps (paper caps). Common fireworks – Chinese crackers, maroon, crackers (atom bomb), palm leaf cracker, flower pot or fountains, rockets. Fancy fireworks-parachute, 7 or 9 or 12 or 14 sounds or mines or salute.

UNIT- V: MILK PRODUCTS

Composition of milk and milk products. Types of milk - Special milks - sterilized milk -flavoured milk - irradiated / vitaminized milk - toned milk-condensed milk. Fermented milks - Cultured butter milk - Acidophilus milk - Yoghurt (Firm-bodied milk). Milk products: Preparation of khoa - gulabjamun - rasagulla and ice cream.

Text Books:

1. Jayashree Ghosh, Fundamental concepts of Applied chemistry, 2006, S. Chand & Company Ltd. New Delhi.
2. P.C. Jain and Monika Jain, Engineering chemistry, Dhanpat Rai & Sons, New Delhi.

Reference Books:

1. B. K. Sharma, Industrial Chemistry Goel Publishing House, 2003, Meerut.
2. Jayashree Ghosh, Text Book of pharmaceutical chemistry 2003 S. Chand and company, New Delhi

FORENSIC CHEMISTRY

(Subject code: 26PCHC2)

Semester: II

ECC-2

Credits: 3

Course Outcome:

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

CO1: examine the crime detection through analytical instruments (K1).

CO2: understand the crime scene (K2).

CO3: apply the techniques for forensic analysis(K3).

CO4: classify the poisons in the living and the dead organisms (K4).

CO5: evaluate the white-collar crimes(K5).

CO6: develop the awareness on Aids - causes and prevention (K6).

UNIT I: Introduction to Forensic Science

Definition – history – facilities offered by various divisions of forensic laboratory expert– relevancy of expert opinion – value of expert evidence.

UNIT II: Scene of occurrence with Physical Evidence

Locard's principle of Exchange – preservation and recording of crime scene - search of evidence. Physical evidence – definition - sources and types of physical evidence – control sample - handling packing , labelling, sealing, forwarding of physical evidence, Chain of evidence – special instruction for special types of exhibits.

UNIT-III: Forensic methods of Analysis

Simple organic analysis – chromatographic techniques – microscopy (comparison of stereoscopic, polarizing and scanning electron microscopy – x-ray diffraction – spectrophotometer. Demonstration: Paper chromatography & TLC to analyse the ink.

UNIT - IV : Alcohol, Narcotics and Poisons

Alcohol and their effects on the body, collection of samples – drunken driving – determination of alcohol – Drug addiction – identification of drug addict – characteristics of drugs (Depressants, stimulants, Hallucinogens) – Toxicology - classification of poison – action of poison on body.

UNIT -V : White Collar Crimes

Characteristic of white collar crimes – classification and forensic investigation of white collar crimes – Cyber crimes – mode and manner of committing cyber crime.

Reference Books:

1. Nabar B S, Forensic Science, SVP national police academy, Hyderabad.
2. Eckert G. William – Introduction to Forensic Sciences, CRC Press, Second Edition
3. Nanda and Tewari – Forensic Science in India A Vision for the 21st Century, Select Publisher, 2001.
4. Saferstein Richard, Criminalistics – An Introduction to forensic science, Prentice Hall , Fifth Edition.

Health Chemistry
(Subject code: 26PCHEC3)

Semester: III

ECC-3

Credits: 3

Course Outcomes:

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

CO1: Recall the basic biological and pharmacological interactions by using both natural products and total synthesis of bioactive molecules (K1).

CO2: demonstrate basic first aid skills needed to control bleeding, ill or injured person and immobilize injuries (K2).

CO3: develop skills to provide one- and two- person cardiopulmonary resuscitation to infants, children and adults (K3).

CO4: Compare the digestion and absorption of carbohydrates, processes involved in their metabolism and regulation of blood sugar (K4).

CO5: deduce the different types of blood lipid, discuss the metabolism of fatty acids and analyze the factors influencing the absorption of cholesterol (K5).

CO6: compile the function and properties of blood, bile pigments and bile acids (K6).

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, Muscle Relaxants, 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-Digestion on 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 - *Adathoda Vasica*, *Hibiscus Rosasinensis*, *Cynodondactylon*, *Tinospora cordifoli*

Reference Books:

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 Eastern Limited, New Delhi, (1993).
5. Alex V Ramani, Food Chemistry, MJP Publishers, Chennai, (2009).

ENVIRONMENTAL CHEMISTRY

(Subject code: 26PCHEC4)

Semester: IV

ECC-4

Credits: 3

COURSE OUTCOMES:

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

CO1: describe the effect of toxic elements on environmental and biological systems (K1).

CO2: demonstrate the knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil (K2).

CO3: Identify the different types of toxic substances & responses and analyse toxicological information(K3).

CO4: analyse the chemical processes involved in different environmental problems (air, water & soil) (K4).

CO5: appraise experimental methods for analysis of water and soil analysis and pollution awareness to society (K5).

CO6: predict the pollutions from diffract industry, pesticides and microorganism (K6).

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, Acid rain, Oxygen and ozone chemistry, Catalytic decomposition process of ozone Concept of atmospheric aerosol Chemistry, Greenhouse 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, chemical fertilizers.

Reference Books:

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

Value Added Course

FUNDAMENTALS IN PHYTOCHEMISTRY

(Subject code: 26PCHVA1)

Semester: II

VA-1

Credits: 3

Course outcome

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

CO1: Grasp the basic principles of Extraction methods (K1).

CO2: understand the separation methods and purification strategies involved in isolation of plant materials. (K2).

CO3: analyze the principles, concepts of phytochemistry and be able to relate with other fields like agriculture and pharmacology (K3).

CO4: detects the phytoconstituents using spectroscopic techniques. (K5).

CO5: Create a method to isolate selected phytoconstituents from the plant source (K6).

Unit 1: Methods of Extraction and Isolation: (6 Hrs)

Maceration, Percolation, Hot extraction. Continuous Soxhlet extraction and Super critical fluid extractions - its advantage and disadvantages. Special extraction methods - Microwave assisted extraction and Ultra sound extraction.

Unit 2: Methods of separation: (6 Hrs)

General introduction to separation techniques- liquid-liquid partition technique, solid-liquid partition methods. Chromatographic techniques – Paper – ascending and descending chromatography, Thin layer chromatography - radial chromatography and HPTLC, Column chromatography - Flash chromatography, HPLC and UPLC.

Unit 3: Identification of Phytoconstituents using spectroscopic methods: (6 Hrs)

Methods of identifications- UV spectroscopy- chlorophyll, Cytochromes, anthocyanin and betacyanin and carotenoids. IR spectroscopy- stretching frequency of alkenes, aromatics, carbonyl groups, amines, cyanides and carboxylic acids. Mass spectroscopy- fragmentation peak and molecular ion peak and NMR spectroscopy chemical shifts and factors depends on chemical shifts of aromatics, hydroxyl groups and implication of NMR spectra.

Unit 4: Important Phytoconstituents: (6 Hrs)

Steroids, Terpenoids- isoprene units, Monoterpenes, sesquiterpenes diterpenes, triterpenes and tetraterpenes and its any two importance in drug discovery. Alkaloids- introduction, classification and its therapeutic and toxicological properties. Introduction to Flavonoids, Tannins, saponin, Essential oil, resin and glycosides.

Unit 5: Modern trends in Phytochemistry and Isolation:**(6 Hrs)**

Ethnopharmacology and drug design from Indian traditional medicinal plants. Relationship of phytochemistry with agriculture, pharmacology and ecology. Extraction of oil of cloves, Isolation of Tannin.

TEXT BOOKS

1. Ahmad, A. & Aqil, F., Phytochemistry: Fundamentals, Modern Techniques, and Applications
2. Harborne, J.B., Introduction to Phytochemistry
3. Online databases like Kew's Medicinal Plant Database for practical exercises.