BHARATHIDASAN UNIVERSITY TIRUCHIRAPPALLI - 620 024.

M.Sc. CHEMISTRY: CHOICE BASED CREDIT SYSTEM - LEARNING OUTCOMES BASED CURRICULUM FRAMEWORK (CBCS - LOCF)

(Applicable to the candidates admitted from the academic year 2026-27 onwards)

Sem.	Courses	Title	Credit	Exam. Hrs	Marks		Total
					Int.	Ext.	
I	Core Course I (CC)	Inorganic Chemistry I	5	3	25	75	100
	Core Course II (CC)	Organic Chemistry I	5	3	25	75	100
	Core Course III (CC)	Physical Chemistry I	5	3	25	75	100
	Core Practical I (CP)	Inorganic Chemistry Practical	4	6	40	60	100
	Elective Course I (EC)	Analytical Chemistry	3	3	25	75	100
		Total	**22**	**-**	**-**	**-**	**500**
II	Core Course IV (CC)	Physical Chemistry II	5	3	25	75	100
	Core Course V (CC)	Inorganic Chemistry II	5	3	25	75	100
	Core Course VI (CC)	Organic Chemistry II	5	3	25	75	100
	Core Practical II (CP)	Organic Chemistry Practical	4	6	40	60	100
	Elective Course II (EC)	Solid State Chemistry	3	3	25	75	100
	Non-Major Elective Course I		2	3	25	75	100
		Total	**24**	**-**	**-**	**-**	**600**

SUMMARY OF CURRICULUM STRUCTURE OF PG PROGRAMMES

Sl. No.	Types of the Courses	No. of Courses	No. of Credits	Marks
1.	Core Courses	11	55	1100
2.	Core Practicals	3	12	300
3.	Elective Courses	3	09	300
4.	Project	1	10	100
5.	Non-Major Elective Courses	2	04	200
	Total	**20**	**90**	**2000**

Instruction hours for these courses is 30 hours.

PROGRAMME OBJECTIVES

- To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories.
- To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.
- To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, Nano science & technology.
- To conduct lesser written tests and to encourage on non-written tests.
- To focus on encouraging students to conduct various academic activities like midterm tests, online tests, open book tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

PROGRAMME OUTCOMES

- To attain profound Expertise in Discipline.
- To acquire the ability to function in multidisciplinary Domains.
- To achieve the ability to exercise Research Intelligence in investigations and Innovations.
- To learn Ethical Principles and be committed to Professional Ethics.
- To incorporate Self-directed and Life-long Learning.
- To obtain the capability to maneuver in diverse contexts with a Global Perspective.
- To attain Maturity to respond to others.

*****

First Year **CORE COURSE - I** **Semester I**

INORGANIC CHEMISTRY - I

(Theory)

COURSE OBJECTIVES

- To understand the basic concepts of main group elements.
- To learn the theories and mechanism of reactions of metal complexes.
- To study the concepts of photochemistry and its applications.

UNIT – I MAIN GROUP CHEMISTRY

Chemistry of boron – borane, Preparation and Structure of diboranes – classification of silicates - silicones. P-N compounds, linear and cyclophosphazenes – S-N compounds – S_4N_4 and polythiazyl compounds – Ionic model –lattice energy – Born-Lande equation – Kapustinskii equation – high temperature superconductors.

UNIT – II PRINCIPLES OF COORDINATION CHEMISTRY

Studies of coordination compounds in solution – detection of complex formation in solution – stability constants – stepwise and overall formation constants, Factors affecting stability constant. Simple methods (potentiometric, pH metric and photometric methods) of determining the formation constants.

UNIT – III THEORIES OF METAL-LIGAND BOND

Crystal field theory – splitting of d-orbitals under various geometries – factors affecting CFSE - Spectrochemical series – Jahn-Teller distortion – spectral and magnetic properties of complexes – site preferences. Limitations of CFT – ligand field theory – MO theory – sigma- and pi-bonding in complexes – Nephelauxetic effect.

UNIT – IV REACTION MECHANISM IN COORDINATION COMPLEXES

Kinetics and mechanism of reactions in solution – labile and inert complexes – ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions. Trans effect – theory and applications – electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes.

UNIT – V INORGANIC PHOTOCHEMISTRY

Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – various photophysical and photochemical processes of coordination compounds. Unimolecular charge-transfer photochemistry of cobalt(III) complexes – mechanism of CTTM, photoreduction – ligand-field photochemistry of chromium(III) complexes – Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium bipyridyl complex.

UNIT – VI Bonding in Small Molecules (For Continuous Internal assessment only)

Valence Bond (VBT) and Molecular Orbital (MO) Theories - Application to small molecules such as BeCl2, BCl3 and CCl4, SF4, ClF3, BrF3 , BrF5 , IF5, IF7 etc – Bonding in Noble gas compounds – XeCl2, XeF4, XeOF4, XeF6.

REFERENCES

1. M. C. Day, J. Selbin and H. H. Sisler, Theoretical Inorganic Chemistry; Literary Licensing (LLC), Montana, 2012.
2. F. A. Cotton and G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry; 6th Ed., A Wiley - Interscience Publications, John Wiley and Sons, USA, 1999.
3. J. E. Huheey, Inorganic Chemistry; 4th Ed., Harper and Row publisher, Singapore, 2006.
4. A. W. Adamson, Concept of Inorganic Photochemistry; John Wiley and Sons, New York, 1975.
5. S. F. A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum; Academic Publishers, Oxford University Press, New York, 1996.
6. A. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry; R. E. Krieger Pubs, Florida, 1984.
7. J. Ferraudi, Elements of Inorganic Photochemistry; Wiley, New York, 1988.
8. F. Basolo and R. G. Pearson, Mechanism of Inorganic Reactions; 2nd Ed., John Wiley, New York, 1967.
9. R. K. Sharma, Inorganic Reactions Mechanism; Discovery Publishing House,NewDelhi.

*****

First Year **CORE COURSE - II** **Semester I**

ORGANIC CHEMISTRY - I

(Theory)

COURSE OBJECTIVES

- To learn the Nomenclature of Organic Compounds
- To learn stereochemistry of organic compounds.
- To understand the basic concepts of aromaticity.
- To know about oxidation and reducing reagents for organic synthesis.

UNIT – I NOMENCLATURE OF ORGANIC COMPOUNDS, REACTIVE INTERMEDIATES AND ELECTRONIC EFFECTS

Nomenclature of heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur.

Reactive Intermediates: Classical and non-classical carbocations, carbanions-free radicals, carbenes, nitrenes, arynes and singlet oxygen- general methods of generation, detection, geometry, stability and reactivity of these intermediates.

Electronic Effects: Inductive effect - resonance effect – hyper conjugation (Baker-Nathan effect) hydrogen bonding (inter and intramolecular) and steric effects.

UNIT – II METHODS OF DETERMINING REACTION MECHANISMS AND CORRELATION ANALYSIS

Kinetics and non-kinetic methods of determination of reaction mechanisms - Thermodynamic and kinetic aspects of organic reactions ,energy profile diagrams - spectroscopic studies, isotopic effects - intermediate versus transition states - product analysis and its importance - crossover experiments-isotopic labelling studies.

Correlation Analysis: Linear Free Energy Relations-Hammet and Taft equations - significance - applications and limitations - classification of solvents.

UNIT – III STEREOCHEMISTRY I

Optical isomerism - Optical activity and chirality - elements of symmetry - Stereochemistry of overcrowded molecules (ansa compounds, cyclophanes and trans cycloalkenes -Newmann, Sawhorse and Fischer projections - representation and interconversion - Absolute configuration – R & S notations for special molecules(allenes, spirans, biphenyls)R-Snomenclature of cyclic chiral compounds - molecules with more than one chiral center - Asymmetric synthesis.

UNIT – IV STEREOCHEMISTRY II

Geometrical isomerism : E and Z nomenclature - determination of configuration of geometrical isomers - configuration of cyclic and bicyclic ring systems - cis- trans nomenclature of three, four and six membered substituted cyclic systems-decalins.

Dynamic Stereochemistry: Quantitative correlation between conformation and reactivity - Winstein-Eliel equation – Curtin- Hammet principle- conformation, reactivity and mechanism of cyclic systems and fused (decalin) ring systems-bridged(norbornane) systems-saponification of an ester - chromic acid oxidation of cyclohexanols - neighbouring group participation.

UNIT – V AROMATICITY AND REAGENTS IN ORGANIC SYNTHESIS

Aromaticity: Aromatic character: Five-, six-, seven-, and eight-membered rings-other systems with aromatic sextets – Huckel's theory of aromaticity,Craig's rule- concept of homoaromaticity and antiaromaticity. – NMR concept of aromaticity and antiaromaticity-non benzeniod aromatic compounds- systems with 2,4,8 and 10 electrons, systems of more than 10 electrons (annulenes), Mobius aromaticity - fullerenes.

Reagents in organic synthesis: Oxidation: Baeyer-Villiger, Jacobsen epoxidation, Shi epoxidation, Jones reagent, DMP, TPAP, NOCl, Mn(OAc)3, Swern oxidation. Reduction: $LiAlH_4$ and $NaBH_4$.

UNIT – VI NAMEREACTIONS AND APPLICATIONS IN ORGANIC SYNTHESIS (For Continuous Internal Assessment Only)

Bamford-Stevens reaction – Barton-McCombie reaction (Barton Deoxygenation) – Baylis-Hillman reaction – Biginelli reaction – Corey-Chaykovsky reaction – Enamines and selective mono- and dialkylation via enamine reactions Henry reaction – Hosomi-Sakurai reaction – Hunsdiecker reaction – Julia olefination and its modifications – Mitsunobu reaction.

REFERENCES

1. R. Panico, WH. Powell, L. Jean, C.Richer, A Guide of IUPAC Nomenclature of Organic Compounds, 1993.
2. R.S. Cahn and O.C. Dermer, Introduction to Chemical Nomenclature, 5th Edn.,Butterworths, 1997.
3. I. L. Finar, Organic Chemistry; Vol.II, 7th Ed., Pearson education Ltd, New Delhi, 2009.
4. J. March, "Advanced Organic Chemistry: Reactions, Mechanisms and Structure",4th ed., Wiley, 1992.
5. R.K. Bansal, "Organic Reaction Mechanisms", Tata McGraw Hill, 1975.
6. P. S. Kalsi, "Organic Reactions and their Mechanisms", New Age International Publishers.
7. E.L.Eliel, "Spectrochemistry of Carbon Compounds", McGraw Hill, 1962.
8. D. Nasipuri, Stereochemistry of Organic Compounds.
9. I.L. Finar, "Organic Chemistry", Vol.II, 5 th ed., ELBS 1975.
10. 10.R.T. Morrison and R.N.Boyd, "Organic Chemistry", 6 th ed., Allyn and Eacon,
11. F.A. Carey and R.J. Sunberg, "Advanced Organic Chemistry, Parts A & B, Plenum, 1984.

*****

First Year **CORE COURSE - III** **Semester I**

PHYSICAL CHEMISTRY - I

(Theory)

COURSE OBJECTIVES

- To study the theories of kinetics, photochemistry and radiation chemistry.
- To understand the concepts of quantum mechanics and group theory.
- To learn the statistical thermodynamics.

UNIT – I CHEMICALKINETICS I

Theories of reaction rate based on statistical mechanics –statistical mechanics and chemical equilibrium - transmission coefficient- reaction coordinate – potential energy surfaces – kinetic isotope effect – Hinshelwood theory – Kassel, Rice and Ramsperger theory (KRRT) – Slater's treatment.

Principle of microscopic reversibility – steady-state approximation – chain reactions: thermal and photochemical reactions between hydrogen and halogens – explosions and hydrogen-oxygen reactions.

UNIT – II FAST REACTION TECHNIQUES, PHOTOCHEMISTRY AND RADIATION CHEMISTRY

Introduction – flow methods (continuous and stopped flow methods) – relaxation methods (T and P jump methods) – pulse techniques (pulse radiolysis, flash photolysis).

Photophysical processes of electronically excited molecules – Jablonskidiagram Stern-Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometers – lasers and their applications.

Differences between radiation chemistry and photochemistry – radiolysis of water, solvated electrons – definition of G value, Curie, linear energy transfer (LET) and Rad – use of dosimetry and dosimeters in radiation chemistry – applications of radiation chemistry.

UNIT– III BASIC QUANTUM MECHANICS

Inadequacy of classical mechanics – black body radiation – Planck's quantum concept – photoelectric effect – wave-particle dualism – uncertainty principle – decline of old quantum theory.

Schrödinger equation – postulates of quantum mechanics – operator algebra: linear operator, Hermitian operators, eigenfunctions and eigenvalues, angular momentum operator – orthogonality and normalization.
Applications of wave mechanics to simple systems – particle in one and three dimensional box.

UNIT – IV STATISTICALTHERMODYNAMICS

Thermodynamic probability – probability theorems – relation between entropy and probability (Boltzmann-Planck equation), ensembles, phase space, Ergodic hypothesis, microstates and macrostates, Maxwell-Boltzmann distribution law. partition functions – translational, rotational, vibrational and electronic partition functions.

Relationship between partition functions and thermodynamic properties – calculation of equilibrium constants from partition functions – heat capacities of monatomic crystals – Debye theory.

Quantum statistics – Bose-Einstein (B.E) and Fermi-Dirac (F.D) distribution equations – comparison of B.E and F.D statistics with Boltzmann statistics – applications of F.D to electrons in metals and B.E to Planck's radiation law.

UNIT– V GROUP THEORY AND ITS APPLICATIONS

Symmetry and group theory: Symmetry elements and operations – point groups – assignment of point groups to molecules – group postulates and types of groups – group multiplication tables, sub groups, similarity transformations – conjugate elements and classes.

Matrix representation of symmetry operations and point groups – reducible and irreducible representations – properties of irreducible representation.

The great orthogonality theorem – construction of character table (C_2V & C_3V)– direct product. Application to vibrational spectra – selection rules for fundamental vibrational transition – IR and Raman activity of fundamentals in H_2O.

UNIT – VI COLLOIDS AND MICELLES **(For Continuous Internal Assessment Only)**

Colloids: Distinction between suspension, colloidal solutions and true solutions – lyophilc and lyophobic colloids – Tyndall effect – stability of colloids – coagulation – emulsions – various types. Micelles: Surfactant (amphipathic molecules) – micellization - critical micelle concentration – size of micelle – aggregation number – Thermodynamics of micellization– reverse micelles.

REFERENCES

1. F. A. Cotton, Chemical Applications of Group Theory; 3rd Ed., John Wiley and Sons, Singapore, 2003.
2. R. L. Flurry, Jr, Symmetry Groups: Theory and Chemical Applications; Prentice Hall, New Jersy, 1980.
3. S. F. A. Kettle, Symmetry and Structure; 2nd Ed., John Wiley and Sons, Chichester, 1995.
4. A.K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.
5. D. A. Mcquarrie, Quantum Chemistry; University Science Books, Sausalito, 2008.

6. I. N. Levine, Quantum Chemistry; 5th Ed., Prentice Hall, New Jersey, 2000.
7. R.K. Prasad, Quantum Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2014.
8. K. J. Laidler, Chemical Kinetics; 3rd Ed., Tata McGraw Hill, Noida, 1987.
9. J. W. Moore and R. G. Pearson, Kinetics and Mechanism; 3rd Ed., John Wiley and Sons, New York, 1981.
10. M. Mortimer and P. G. Taylor, Chemical Kinetics and Mechanism; 1st Ed., Royal Society of Chemistry, UK, 2002.
11. J. N. Gurtu and A. Gurtu, Advanced Physical Chemistry; 5th Ed., PragathiPrakashan, Meerut, 2006.
12. J. I. Steinfeld, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics; 2nd Ed., Prentice Hall, New Jersey, 1999.
13. K. S. Gupta, Chemical Kinetics and Reaction Mechanism; RBSA Publishers, Jaipur, India, 1992.
14. P. W. Atkins, Physical Chemistry; 7th Ed., Oxford University Press, Oxford, 2001.
15. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry - Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
16. HoriaMetiu, Physical Chemistry, Thermodynamics; Taylor and Francis, Singapore, 2006.
17. K. K. Rohatgi-Mukherjee, Fundamentals of Photochemistry; 3rd Ed., New Age International Pvt. Ltd., New Delhi, 2014.
18. J. W. T. Spinks and R. J. Woods, Introduction to Radiation Chemistry; 3rd Ed., John Wiley and Sons, New York, 1990.

*****

First Year **CORE PRACTICAL - I** **Semester I**

INORGANIC CHEMISTRY PRACTICAL

(Practical)

COURSE OBJECTIVES

- To perform the semi-micro qualitative analysis.
- To estimate the metal ions using colorimeter.
- To Prepare the coordination complexes

1. **Semi-micro qualitative analysis** of a mixture containing two common cations (Pb, Bi, Ca, Cd, Fe, Cr, Al, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, NH_4) and two less common cations (W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U, Li).

2. **Photoelectric colorimetric estimation** of copper, ferric, nickel, chromium and manganese ions

3. **Preparation of complexes**

    1. Tris(thiourea)copper(I) chloride
    2. Tetraamminecopper(II) sulphate
    3. Potassium trisoxalatoferrate
    4. Potassium trisoxalatoaluminate(III)
    5. Potassium trisoxalatochromate(III)
    6. Hexamminecobalt(III) chloride

REFERENCES

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rd Ed., National Pubs, London, 1988.
2. G. Svehla, Text Book of Macro and Semimicro Qualitative Inorganic Analysis; 5thEd., Longman group Ltd, London, 1987.
3. A. I. Vogel, Text Book of Quantitative Inorganic Analysis;6th Ed., Longman, New Delhi, 2000.

*****

First Year **ELECTIVE COURSE - I** **Semester I**

ANALYTICAL CHEMISTRY

(Theory)

COURSE OBJECTIVES

1. To learn the instrumental methods
2. To learn the nature of errors and their types.
3. To understand the various techniques in chromatography.
4. To understand the principles and instrumentation of thermoanalytical and fluorescence techniques.
5. To studying detail the electroanalytical techniques.

UNIT – I INSTRUMENTAL METHODS OF ANALYSIS

Principles and applications of extended X-ray absorption fine structure (EXAFS) – surface extended X-ray absorption (SEXAFS) – atomic absorption spectroscopy (AAS) – flame emission spectroscopy (FES) – turbidimetry – theory and applications. Instrumentation and sampling techniques in UV-visible and IR spectroscopy.

UNIT – II DATA AND ERROR ANALYSIS

Various types of error – accuracy, precision, significant figures – the binomial distribution, the Poisson distribution and normal distribution – describing data, population and sample, mean, variance, standard deviation- Hypothesis testing, means t-Test, paired t-Test – analysis of variance (ANOVA) – correlation and regression.

Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – general polynomial equation fitting, linearizing transformations, exponential function fit – r and its abuse – multiple linear regression analysis, elementary aspects.

UNIT – III CHROMATOGRAPHY

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

UNIT – IV THERMOANALYTICAL METHODS AND FLUORESCENCE SPECTROSCOPY

Principles – instrumentations and applications of thermogravimetry analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) – thermometric titrations – types – advantages.

Basic aspects of synchronous fluorescence spectroscopy – spectral hole burning – flow cytometry – fluorometers (quantization) – instrumentation – applications.

UNIT – V ELECTROANALYTICAL TECHNIQUES

Polarography – principles and instrumentation – dropping mercury electrode – advantages –Ilkovic equation – polarographic maxima – cyclic voltammetry – chronopotentiometry – amperometric titrations: principles – techniques – applications.

Electrochemical sensors, ion-sensitive electrodes, glass – membrane electrodes, solid-liquid membrane electrodes – ion-selective field effect transistors (ISFETs) – sensors for the analysis of gases in solution.

UNIT – VI TYPES OF TITRATIONS (For Continuous Internal Assessment Only)

Redox titration: Redox potentials, theory and feasibility of redox titration, calculation of potentials at different stages of titrations, redox indicators, their choice and applications. Precipitation titrations: Theory and types, Mohr, Volhard and Fajan's methods. Adsorption indicators: theory, choice and applications. Complexometric titrations: Theory, Stepwise and overall formation constants, Titrations involving chelates (EDTA). Metallochromic indicators: Theory and Choice, Masking and demasking methods and applications.

REFERENCES

1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry; Oxford University Press, UK, 2006.
2. J. Topping, Errors of Observation and Their Treatment; 4th Ed., Chapman Hall, London, 1984.
3. A. Braithwaite and J. F. Smith, Chromatographic Methods; 5th Ed., Springer, Germany; 1995.
4. V. K. Srivastava and K. K. Srivastava, Introduction to Chromatography; 2nd Ed., Holden Day, New York, 1985.
5. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis; 6th Ed., CBS Publishers and Distributors, Chennai, 1986.
6. D. A. Skoog, D. M. West and D. J. Holler, Fundamentals of Analytical Chemistry, 7th Ed., Harcourt College Publishers, Singapore, 2004.
7. A. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy; Wiley-Interscience, New York, 1999.
8. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy; 4th Ed., Tata McGraw-Hill, New Delhi, 1994.
9. A. I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman, New Delhi, 2000.
10. D. C. Harris, Quantitative Chemical Analysis; 4th Ed., W. H. Freeman Publications, New York, 1995.
11. S. C. Gupta, Fundamentals of Statistics; 6th Ed., Himalaya Publications, Delhi, 2006.

*****