VIJAYANAGARA SRI KRISHNADEVARAYA UNIVERSITY

JNANASAGARA CAMPUS, BALLARI-583105

Department of Studies in Industrial Chemistry

Programme: Master of Science (M.Sc.) in Industrial Chemistry

Duration: 2 Year (4 semesters)

Programme Overview:

Master of Science (M.Sc.) in Industrial Chemistry programme is designed to prepare students for a career in teaching, research or industry by introducing them to a wide range of concepts in industrial chemistry and training in techniques applicable in various research areas. The programme also aims to provide basic understanding of principles & concepts of industrial chemistry through well structured teaching-leaning process and experimentation to understand the new dimensions of industrial chemistry.

Programme Educational Objectives (PEOs):

After 3-4 years of completion of the programme the graduates will be able to:

4. Demonstrate competency in industrial chemistry to solve and anaylse contemporary problems.
5. Demonstrate research skills which might include laboratory techniques, numerical techniques and computer programming.
6. Occupy positions in academic/research institutions / industry.
7. Demonstrate leadership qualities to achieve professional and organizational goals with commitment to ethical standards and team spirit.

Programme Outcomes (POs):

After earning the post graduate degree in Industrial Chemistry the student will be able to;

1. Interpret, with strong foundation, the concepts of chemistry including inorganic, organic, physical, analytical, pharmaceutical, polymer, petroleum, dyes, medicinal and material science.
2. Implement the proper procedures and regulations for safe handling and use of chemicals and can follow the proper procedures and regulations for safe handling when using chemicals

3. Use modern instrumentation and classical techniques, to design experiments, properly record the results of the experiments and analyze the results
4. Use modern library searching and retrieval methods to obtain information about a topic, chemical, chemical technique, or an issue relating to chemistry
5. Develop skills of chemical engineering including unit operation, unit processes, reactor designing, process calculation, process control.
6. Identify and solve the challenges related to chemistry in the industry.
7. Communicate the results of their work, effectively, both verbally and in writing to chemists and non-chemists.
8. Understand the philosophical, and global environmental dimensions of problems and issues facing chemists in the social context.
9. Acquire enough confidence in teaching chemistry.
10. Recognize the need to engage in life-long learning
11. Acquire skills for handling the modern analytical instruments
12. Establish small start-up industry related to manufacturing of chemical products
13. Establish analytical laboratory for analysing industrial materials.

VIJAYANAGARA SRI KRISHNADEVARAYA UNIVERSITY

Distribution of Courses/Papers in Postgraduate Programme I to IV Semester as per Choice Based Credit System (CBCS)

INDUSTRIAL CHEMISTRY

M.Sc. I-SEMESTER

Semester No.	Category	Subject code	Title of the Paper	Marks			Teaching hours/week			Credit	Duration of exams (Hrs)
				IA	Sem. Exam	Total	L	T	P		
FIRST	DSC1	21 ICH1 C1 L	Concepts in Inorganic chemistry	30	70	100	4	-	-	4	3
	DSC2	21 ICH1C2 L	Theoretical Organic chemistry	30	70	100	4	-	-	4	3
	DSC3	21 ICH1C3 L	Thermodynamics, Chemical kinetics and Electrochemistry	30	70	100	4	-	-	4	3
	DSC4	21 ICH1 C4 L	Analytical Chemistry	30	70	100	4	-	-	4	3
	SEC1	21 ICH1 S1 LP	Computational Chemistry	20	30	50	1	-	2	-	4
	DSC1P	21 ICH1 C1 P	Inorganic Chemistry Practicals	20	30	50	-	-	4	2	4
	DSC2P	21 ICH1 C2 P	Organic Chemistry Practicals	20	30	50	-	-	4	2	4
	DSC3P	21 ICH1 C3 P	Analytical Chemistry Practicals	20	30	50	-	-	4	2	4
Total Marks for I Semester						**600**				**24**	

II-SEMESTER

Semester No.	Category	Subject code	Title of the Paper	Marks			Teaching hours/week			Credit	Duration of exams (Hrs)
				IA	Sem. Exam	Total	L	T	P		
SECOND	DSC5	21 ICH2C5L	Coordination Chemistry	30	70	100	4	-	-	4	3
	DSC6	21 ICH2C6L	Chemistry of Natural products, Reagents in Organic synthesis and Heterocyclic Compounds	30	70	100	4	-	-	4	3
	DSC7	21 ICH2C7L	Electro and Photochemistry	30	70	100	4	-	-	4	3
	DSC8	21 ICH2C8L	Instrumental methods of analysis	30	70	100	4	-	-	4	3
	SEC2	21 ICH2 S2 P	Research Methodology	20	30	50	1	-	2	2	2
	DSC 5P	21 ICH2 C4 P	Synthesis of Coordination compounds	20	30	50	-	-	4	2	4
	DSC6P	21 ICH2 C5 P	Organic synthesis	20	30	50	-	-	4	2	4
	DSC7P	21 ICH2 C6 P	Instrumental methods of analysis	20	30	50	-	-	4	2	4
Total Marks for II Semester						**600**			**600**		

III-SEMESTER

Semester No.	Category	Subject code	Title of the Paper	Marks			Teaching hours/week			Credit	Duration of exams (Hrs)
				IA	Sem. Exam	Total	L	T	P		
THIRD	DSC9	21 ICH2 C9 L	Spectroscopy	30	70	100	4	-	-	4	3
	DSC10	21 ICH2 C10 L	Unit Operations	30	70	100	4	-	-	4	3
	DSE1	21ICH3 E1AL	A.Polymer Chemistry	30	70	100	4	-	-	4	3
		21ICH3 E1BL	B. Water Management in Industries								
		21ICH3 E1CL	C. Quality control and environment, health and Safety measures								
	DSE2	21ICH3E2AL	A. Industrial materials	30	70	100	4	-	-	4	3
		21ICH3E2BL	B. Industrial Management and Pollution monitoring and control								
		21ICH3E2CL	C. Chemical Analysis in Agro, Food and Pharmaceutical Industries								
	GEC1	21ICH3G1AL	A.Green Chemistry	20	30	50	2	-	-	2	2
		21ICH3G1BL	B.Metals in Medicine and Anticancer Agents								
		21ICH3G1CL	C.Adsorption and Surface Phenomena								
	SEC3	21 ICH3S3 LP	Instrumental methods of Analysis	20	30	50	1	-	2	2	2
	DSC9P	21 ICH3 C7 P	Interpretation of Spectra of the compounds	20	30	50	-	-	4	2	4
	DSE2P	21 ICH3 E2 P	Analysis of Industrial Materials	20	30	50	-	-	4	2	4
Total Marks for III Semester						**600**				**24**	

IV-SEMESTER

Semester No.	Category	Subject code	Title of the Paper	Marks			Teaching hours/week			Credit	Duration of exams (Hrs)
				IA	Sem. Exam	Total	L	T	P		
FOURTH	DSC11	21 ICH 4C11L	Inorganic Industrial materials	30	70	100	4	-	-	4	3
	DSC12	21 ICH 4C12L	Unit Processes	30	70	100	4	-	-	4	3
	DSE3	21ICH 4E3AL	A. Pharmaceutical Industrial Chemistry	30	70	100	4	-	-	4	3
		21 ICH 4E3BL	B. Advanced Topics in Chemistry								
		21 ICH 4E3CL	C. Manufacturing of Common Materials								
	DSE4	21ICH 4E4AL	A. Environmental Impact Assessment	30	70	100	4	-	-	4	3
		21 ICH 4E4BL	B. Food Industry and Agrochemicals								
		21 ICH 4E4CL	C. Chemistry in Biology								
	GEC2	21ICH4 G2AL	A.Water Harvesting and Renewable Energy Sources	20	30	50	2	-	-	2	2
		21ICH4 G2BL	B.Basics of Chemistry								
		21ICH4 G2CL	C.Impact of Chemical Fertilizers and Pesticides on Agriculture								
	DSC11P	21 ICH4 C11 P	Analysis of Inorganic Materials	20	30	50	-	-	4	2	4
	Project	21 ICH 4C1R	In-plant Training/ Research Project	30	70	100	-	-	4	4	4
Total Marks for IV Semester						**600**				**24**	

(I-IV semester)- Total Marks: 2400 and Total credits: 96

DSC – Department Specific Core, DSE – Discipline Specific Elective, SEC – Skill Enhancement Course, GEC – Generic Elective Course, IA – Internal Assessment, SEE – Semester End Examination, L – Lecture, T – Tutorial, P – Practical.

M.Sc. First Semester

Course: Concepts in Inorganic Chemistry	**Course Code:** 21 ICH1 C1 L
Teaching Hours/Week (L-T-P): 4 - 0 - 0	**No. of Credits:** 04
Internal Assessment: 30 Marks	**Semester End Examination:** 70 Marks

Course Objectives:

1.The objective of this course is to refresh the chemistry knowledge learnt in earlier programs and to introduce some advanced concepts on related topics.

Unit I :Review of periodic properties and theories of Bonding [13 hrs]

Review of periodic properties- Atomic size, ionization potential, electron affinity and electro negativity.

Ionic Bond:

Radius ratio rules, types and structures of simple ionic compounds, lattice energy, Born-Lande equation, Kapustinskii equation, Size effects, polarizing power and polarizability of ions, Fajan's rules, solubility of ionic solids and hydration energy.

Covalent Bond and Metallic Bond:

VSEPR theory shapes of molecules-ClF3, ICl4-, TeF5-, I3-, TeCl62-, XeF6, SbCl63-, IF7, XeF82-, TaF83-; Concepts of hybridization, Energetics of hybridization, Bent rules and energetics of hybridization, partial ionic character, covalent-coordinate and multicentre bonding, M.O theory-LCAO approach, σ, δ and π molecular orbits. M.O treatment of homo nuclear and hetero nuclear diatomic molecules, Bond order in delocalized π- bonding systems, Ex: CO32-, NO3- and SO3. Metallic bonding – electron sea model, VBT. Hydrogen Bonding

UNIT II : Band theory of Solids [10 Hours]

Semi conductors – Bonding and conductivity, mechanism of conductivity, energy bands in semi-conductors, impurity conductors, p-n and n-p-n junctions. Importance of semiconductors. Super conductors – occurrence of super conductivity, its destruction by magnetic fields, effect of IR and isotope effect, BCS theory of super conductivity, applications.

Defects in solids – Frenkel and Schotky defects and chemical reaction of solids.

Unit III :Concepts of Acids and Bases [10 Hours]

Introduction different definitions, types of reactions, solvent systems and leveling effect. Generalized acid-base concept-basicity of metal oxides, hydration and hydrolysis. Measurement of acid – base strengths. Steric affects-back strain, front strain and internal strain. Solution effects with respective to liquid ammonia, anhydrous sulphuric acid, acetic acid and liquid sulphur dioxide, acetic acid, HF, N2O4, super acids and molten salts. HSAB-classification & strength of hardness and softness. Irving-William's series. Theoretical bases of hardness and softness.

Unit IV : Organometallic chemistry [10 Hours]

Classification & nomenclature of organometallic compounds – 16 & 18 electron rules – electron counting by neutral atom & oxidation state method.

Organometallic compounds of main group elements:- General methods of synthesis structure and bonding in alkyls of Li, Mg, & Al.

Transition Metal alkyls (synthesis and stability), Synthesis structure and bonding in metal olefins, carbonyls, nitrosyls, carbenes and metallocenes. Isobolality and Fluxionality

Unit V : Reactions and Catalytic applications of Organometallic Compounds [10 Hours]

Fundamental reactions: Substitution in carbonyl complexes, Mechanisms, Insertion reactions, CO, SO2, olefin insertions, oxidative additions, one electron, addition of oxygen, reductive elimination, CH activation, Use of Organometallic Compounds as catalysts – Catalytic behaviour – Homo catalysis –. Anchoring of Catalysts

Hydrogenation. Hydrogenation of olefins (oxo reaction-cobalt and rhodium oxo catalysts), carbonylation of alcohols – Monsanto acetic acid process, Wacker process. Polymerization of olefins and acetylenes: Ziegler – Natta catalysis systems. Fischer – Tropsch reaction, Water Gas Shift reactions.

Reference :

1. J. E. Huheey, E. A. Keiter and R.L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education, 2004.
2. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, John Wiley & Sons, Inc., New York, 2009.
3. J. D. Lee, Concise Inorganic Chemistry, Blackwell Science, Oxford, 2000.
4. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Shriver &Atkins:Inorganic Chemistry, Fourth edition, Oxford University Press, Oxford, 2000.
5. F. A. Carey G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience, 2003.
6. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Prentice Hall, 2005
7.Chemistry of Elements – N.N. Greenwood and A.Earnshaw, Pergaman (2000).
8. Inorganic Chemistry – 2nd edition, C.E Housecraft and A.G Sharpe, Pearson Education Ltd. (2005).
9. Inorganic Chemistry – 2nd edition, D.F Shriver, P.W.Atkins and C.H.Langtore Oxford University Press (1994).
10. Concepts and Models of Inorganic Chemistry – 3rd edition, B.E Douglas, D.H. Mc Daniel and Alexander, Wiley (2001)

Course Outcomes (CO): After the completion of this course, the student would be able to;

CO	Statement
1	Illustrate and explain the atomic structure.
2	Relate the quantum numbers and atomic orbitals and their shapes.
3	Evaluate and relate the periodic properties of elements based on electronic configuration.
4	Explain the structure and bonding in molecules and predict the structures of molecules.
5	Explain selected crystal structures and the parameters that affect the crystal structure of a compound and perform calculations of the lattice enthalpy of ionic compounds.
6	Differentiate bonding in metals from their compounds.
7	Explain the structures in solids and identify the reasons for differences in electrical properties.
8	Explain the definitions of acids / bases based on different theories and predict the reactions between acids and bases.
9	Identify the difference between a coordination and organometallic compound based on the nature of bonding and chemical properties.
10	Depict the nature of M--C bond in different organometallic compounds which determines their properties.

11	Explain different types of reactions of organometallic compounds with their mechanisms.
12	Explain various applications of organometallic compounds in chemical industries as catalysts

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Course: Theoretical Organic chemistry	**Course Code:** 21 ICH1 C2 L
Teaching Hours/Week (L-T-P): 4 - 0 - 0	**No. of Credits:** 04
Internal Assessment: 30 Marks	**Semester End Examination:** 70 Marks

Course Objectives:
1.The objective of this course is to make the students to get acquainted with some new concepts and topics in organic chemistry.

Unit I : Concept of Resonance and Aromaticity [11 Hours]
Concept of resonance, Delocalized chemical bonding: Conjugation, cross conjugation,. Aromaticity. Huckel's rule of aromaticity.Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Antiaromaticity. Aromaticity in benzenoids, meso-ionic compounds. Nonaromaticity of organic systems(3-7 membered rings & ring ions). Homo-aromaticity. Alternant and nonalternant hydrocarbons, Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion. Hyperconjugation. Tautomerism

Unit II : Stereochemistry of Organic compounds [11 Hours]
Elements of symmetry, concepts of chirality, optical isomerism, projection formulae, Fisher, Saw horse, Newman and Flying wedge formulae and their inter conversion, optical isomerism due to one or more than one chiral centres.
Threo and erythro isomers, enantiomers, diastearic isomers and epimers. D-L and R-S conversions. Optical activity in the absence of chiral carbon – Biphenyls, allenes and spiranes, optical isomerism of nitrogen compounds , conformational analysis of (cyclic and acyclic systems) – ethane, propane, butane, mono &disubstitedcyclohexanes.
Geometrical isomerism – cis-trans, syn-anti and E-Z nomenclature, isomerism in ketoximes and aldoximes, Beckmann rearrangement.

Unit III : Reaction mechanisms, and Reaction intermediates [11 Hours]

Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals,carbenes and nitrenes.
Classification of reactions and mechanisms. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.
Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, from stereochemical evidence.
Effect of structure on reactivity:- Resonance and field effects; steric effects. Nucleophilic substitution reaction at a saturated carbon: SN1, SN2, and SET mechanisms. Effect of substrate structure, attacking nucleophile, leaving group.Ambident nucleophiles and substrates

Unit IV : Named Reactions [12 Hours]

1 Acetoacetic ester synthesis 2 Aldol condensation 3 Alkene metathesis 4 Bayer-Villiger oxidation 5 Birch reduction 6 Claisen condensation 7 Claisen rearrangement 8 Clemmensen reduction 9 Cope rearrangement 10 Dieckmann condensation 11 Diels-Alder reaction 12 Friedel-Crafts reaction 13 Gabriel synthesis 14 Grignard reaction 15 Heck coupling 16 Hydroboration reaction 17 Malonic ester synthesis 18 Mannich reaction 19 Michael addition 20 Ozonolysis 21 Sharpless Dihydroxylation 22 Sharpless Epoxidation 23 Simmons-Smith reaction 24 Sonogashira coupling 25 Stille coupling 26 Strecker synthesis of amino acids 27 Suzuki coupling 28 Wadsworth-Emmons reaction 29 Williamson ether synthesis 30 Wittig reaction

Unit V: Pericyclic Reactions [11 Hours]

Definition, classifications of pericyclic reactions. Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1.3.5-hexa triene and allyl systems. Woodward and Hoffmann correlation diagram. FMO & PMO approach, electrogatic reactions-conrotator and disrotatory motions, 4n, 4n+2 and allyl systems.
Cycloaddition – antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes. 1, 3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements, superfacial and antrafacial shifts of H., shifts involving carbon moieties, 3, 3-and 5, 5 – sigmatropic rearrangements, claisen, cope and azo cope rearrangements.

References:

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Fifth edition, Springer, New York, 2007
2. T. H. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry, Second edition, Harper & Row, New York, 1981
3. N. S. Isaacs, Physical Organic Chemistry, ELBS, Longman, UK, 1987.
4. D. Nasipuri, Stereochemistry of Organic Compounds. Principles and Applications, Second edition, Wiley Eastern Limited, New Delhi, 1994.
5. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
6. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.
7. P. Sykes, Advanced Organic Chemistry; Reaction Mechanisms, Longman and Scientific Technical, New York, 1985
8. R. Brukner,Advanced Organic Chemistry, Reaction Mechanisms, Academic Press, 2002.
9. R. O. C. Norman and J.M. Coxon, Principles of Organic Synthesis, CRC Press, UK, 1993.
10. J. M. Berg, J. L. Tymoczko and L. Stryer, Principles of Biochemistry, 6th edition, W.H. Freeman & Co, 2006.
11. D. L. Nelson and M. M. Cox. Lehninger Principles of Biochemistry, 5th edition, W.H. Freeman & Co, 2008.
12. R. K. Murray, D. K. Granner, P. A. Mayes and V. W. Rodwell, Eds. Harper's Illustrated Biochemistry 26th edition, McGraw Hill, 2003

Course Outcomes (CO): After the completion of this course, the student would be able to;

CO	Statement
1	Explain the importance of resonance concept amongst organic compounds and depict the resonating structures.
2	Interpret and explainthe concept of aromaticity and the main properties of aromatic compounds
3	Figure out the differences among antiaromaticity, nonaromaticity and homoaromaticity.
4	Explain hypercojugation and tautomerism.
5	Classify molecules as chiral or achiral, identify chiral carbons as (R) or (S),
6	Identify relationships between pairs of molecules as enantiomers, diastereomers, or equivalent, and identify when a solution is racemic versus optically active.
7	Recognize and classify fundamental organic reactions such as SN1, SN2, E2, E1, alkene addition, electrophilic aromatic substitution, 1,2/1,4-additions, ring-opening, and radical halogenation.
8	Explain, and apply concepts associated with these general reaction types to product prediction, synthesis design, and reaction mechanism.

9	Write logical and detailed mechanisms for various fundamental reactions of alkanes, halocarbons, alkenes, dienes, and arenes.
10	Design retrosynthetic analysis for efficient multi-step syntheses involving halocarbons, alkenes, and arenes as intermediates or final products

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Course: Advanced Physical Chemistry	**Course Code:**21 ICH1 C3 L
Teaching Hours/Week (L-T-P): 4- 0 - 0	**No. of Credits:** 04
Internal Assessment: 30 Marks	**Semester End Examination:** 70 Marks

Course Objectives:

1.The objective of studying advanced physical chemistry in the first semester of postgraduate programme is to give a essential knowledge of physical chemistry to the students with respect to chemical thermodynamics, reactions in solutions, chemical kinetics, catalysis, electrochemistry and phase rule.

Unit I : Chemical Thermodynamics [12 Hours]

A brief resume of laws of thermodynamics (combined form of 1st and 2nd laws), entropy as a measure of unavailable energy, concept of fugacity and free energy, entropy and free energy changes and spontaneity of processes. Variation of free energy with T & P. Maxwell's relations, thermodynamic equations of state, limitations of Van't Hoff' s equation, Nernst Heat theorem & its applications. Third law of thermodynamics, determination of third law of entropies.

Application of Thermodynamics:

Entropy and free energy of mixing, partial molar quantities, partial molar volume and free energy (chemical potential), their significance and determinations. Gibbs- Duhem and Duham-Margules equations.

Unit II : Chemical Kinetics [12 Hours]

Theories of Reaction Rates:

Activated complex theory and its applications to reactions in solution. Theory of unimolecular reactions- Lindeman, Hinsel-Wood and RRKM theory

Chemical Kinetics:

Complex reactions- parallel, consecutive and reversible reactions. Chain reactions (H2-halogen reactions). Branched chain reactions- general rate expression, explosion limits. Photochemical (H2-halogen reactions) and oscillatory reactions.

Unit III : Electrochemistry [10 Hours]

Electrochemistry of Solutions:

Ionic atmosphere, physical significance of k (Cuppa), Debye-Huckel theory to the problem of activity coefficient, Debye-Huckel limiting law, Debye-Huckel equation for appreciable concentration. The Huckel and Bronsted equation. Qualitative verification of Debye-Huckel equation, Debye-Huckel Onsager conductance equation, Bjerrum theory of ion association-triples ion-conductance minima. Electrical double layer and its thermodynamics. A brief survey of Helmholtz – Perrin, Gouy – Champman and Stern electrical double layer, EMF cells, liquid junction potential and its determination. Energetics of cell reactions, effect of temperature, pressure and concentration on energetics of cell reactions (Calculation of ΔG, ΔH and ΔS)

Unit IV : Catalysis [10 Hours]

Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalyzed reactions. Acid-base catalysis (general and specific), protolytic and phototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalyzed reactions-Michaelis- Menten equation. Effect of pH, temperature & inhibitors. Industrial applications of catalysts.

Surface Reaction Kinetics:

A review of adsorption isotherms, uni- and bi-molecular reactions, multilayer adsorption-BET equation-application in surface area determination. Harkin-Jura equation- application. Desorption & heterogeneous catalysis-catalytic activity at surfaces. Mechanism of surface reactions.

Unit V : Phase Equilibria and Reactions in Solution: [10 Hours]

Introduction and definitions, derivation of phase rule, one component system, two component system, the Nernst distribution law, solid- liquid systems-condensed systems, Alloys, three component systems

Substituent effects on the rates of reactions, linear free energy relationships - Hammett and Taft equations

References:

1. An Introduction to Electrochemistry, S. Glasstone, Van Nostrand, East-West 1965.
2. Modern Electrochemistry, Vol. I and II, 2nd Edition, J. O'M Bockris and A. K. N. Reddy, Plenum, 1977.
3. Electrolytic Solutions, R. A. Robinson and R. H. Stokes, Butterworths, London, 1959.
4. Physical Chemistry, P. W. Atkins, ELBS, 1986.
5. Physical Chemistry, 4 th Edition, Silbey, Alberty, Bawendi, Wiley, India, 2007.
6. Chemical Kinetics, 2nd Edition, K. J. Laidler, TMH.
7. Kinetics and Mechanism, 2nd Edition, A. A. Frost and R. G. Pearson.
8. Physical Chemistry, P. W. Atkins, ELBS, 3rd Edition, 1986.
9. Physical Chemistry, G. M. Barrow, 5th Edition, 2007.
10. Basic Physical Chemistry by W. J. Moore, Prentice Hall, 1986.

Course Outcomes (CO): At the end of the advanced physical chemistry course, student should be able to

CO	Statement
1	Solve the problems related to laws of thermodynamics, write and construct the Maxwell's equations. Summerizethe Equations for free energy change, enthalpy calculations
2	Illustrate the partial molar quantities and free energy change in the mixing of two solutions and chemical potential.
3	Summerize the activated complex theory and theories of unimolecular reaction rates
4	Provide the equations for rate constants of the parallel, consecutive, photochemical, oscillatory and chain reactions
5	Predict the effect of substituents, salt and solvent on reaction rates.
6	Able to visualize thebehaviour of ions in solutions, perform the calculations of activity coefficients
7	Manipulate the catalytic activity and mechanism involved in catalytic activities.
8	Elaborate the kinetic aspects of enzyme catalysed reactions. and indicate the effect of PH

	,temperature and pressure on these reactions
9	Recognize and differentiate between absorption and adsorption phenomenon.
10	Recognize the cause and consequences of electrical double layer
11	Predict the energetics of cell reactions
12	Construct a phase diagram for three component system.

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Course: Analytical Chemistry	**Course Code :** 21 ICH1 C4 L
Teaching Hours/Week (L-T-P): 4- 0 - 0	**No. of Credits:** 04
Internal Assessment: 30 Marks	**Semester End Examination:** 70 Marks

Course Objectives:

1.The objective of this course is to make the students to get familiarized with various analytical techniques and their importance in all the fields of chemistry.

Unit I : Sampling, Errors, and statistical analysis [11 Hours]

Errors and Sampling:

Limitations of analytical methods, classifications of errors, accuracy, precision, minimization of errors, significant figures and computations, mean and standard deviation, distribution of random errors, relativity of results, confidence interval, comparison of results, comparison of the means of two samples, Paired t- test, the number of replicate determinations, correlation and regression, linear regression, comparison of more than two means (analysis of variance), Least square method, 6 sigma concept. Quality control and quality assurance. The basis of sampling, sampling procedure, sampling statistics, sampling and physical state, crushing and grinding, hazards in sampling

Unit II :Titrimetry and Gravimetry [13 Hours]

Acid base titrations: Principle, titration curves for strong acid - strong base, weak acid – strong base, weak base –strong acid, determination of equivalence point – theory acid base indicators, colour change range of indicator, applications for nitrogen, nitrates and carbonates estimation.

Complexometric Titrations: Introduction, a simple complexation titration, titration curves, types of EDTA titrations, titrations of mixtures, selectivity, masking and demasking agents, metal ion indicators, some practical considerations.

Precipitation Titrations: Precipitation reactions, titration curves, factors influencing the sharpness of end points, chemical indicators for precipitation titrations, applications of precipitation titration analysis.

Oxidation –Reduction Titrations: Redox process, titration curves, redox indicators and applications.

Gravimetric analysis:

Requirements & conditions of precipitations, co-precipitation, post precipitation, nature of the precipitate, super saturation, precipitation from homogeneous solution and effect of excess of precipitant, temperature, pH and complex formation on completeness of precipitation. Filtration, washing of precipitates, drying and ignition of precipitates.

Organic Reagents in Inorganic Analysis: Organic precipitants, general properties, reagents as precipitants

UNIT III : Colorimetry and Spectrophotometry [10 Hours]

Characteriztion of Electromagnetic radiations, Colorimetry and Spectrophotometry

Electromagnetic radiation

Characterization – quantization of energy levels – regions of electromagnetic radiation spectrum – interaction electromagnetic radiation with matter – representation of spectra-intensity and width of spectral lines.

Colorimetry and Spectrometry :

Quantitative aspects of absorption – Beer- Lambert's law. Terminology associated with absorption measurements. Criteria for spectrophotometric determinations with examples (Fe, Mo and Ni). Limitations of the law,

Turbidimetry and Nephelometry

Tyndall, Rayleigh and Raman Scattering - Principles, Instrumentation and Applications of Turbidimetry and Nephelometry

Unit IV : Separation Techniques [10 Hours]

Basic separation techniques in analysis, classification

Solvent Extraction:

Principle, distribution law, choice of solvents for extraction, synergic extraction, techniques-batch, continuous and multiple extractions and applications.

Principles of Chromatography:

Distribution coefficient, modes of chromatography, selection of stationary and mobile phases, analyte development and elution. Chromatographic performance parameters-retention time and volume capacity factor, plate height and resolution

Paper and thin layer Chromatography:

General principles and classification of chromatographic methods-paper, thin layer, column and liquid chromatography.

Unit V : Thermal Methods of Analysis [10 Hours]

Thermo Gravimetric Analysis:

Introduction, thermo gravimetric analysis(TGA) – types of thermo gravimetric analysis, principles, factors affecting the results – heating rate, thermobalance, furnace instrument control/data handling. Applications-purity and thermal stability, evaluation of correct drying temperature, analysis of complex mixture and determination of kinetic parameters of thermal degradation.

Differential Thermal Analysis (DTA): Theory , variables affecting the DTA, general principles, instrumentation, applications – analysis of the physical mixtures and thermal behavior study, determination of decomposition point.

Differential Scanning Calorimetry (DSC):

Basic principle, differences between DTA and DSC, instrumentation – power compensated DSC, heat flux DSC, applications – studies of thermal transistors and isothermal crystallization, pharmaceutical industry for testing the purity of the samples. Thermometric titrimetry and direct injection enthalpimetry-principle, instrumentation, applications.

References:

1. Vogel's Text book of Quantitative Chemical Analysis, J. Bassett, G. H. Jeffery and J.Mendham, Pearson, 7th edition, (2009).
2. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co.(1974).
3. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co.,London (1972).
4. Principles of Instrumental Analysis - Skoog, Holler, Nieman, 5th ed., Harcourt CollegePublishers, 1998.
5. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York1994.

Course Outcomes (CO): After the completion of this course, the student would be able to;

CO	Statement
1	Explain the fundamentals of analytical chemistry and differentiate between qualitative and quantitative analyses.
2	Evaluate the analytical data in terms of statistics.
3	Estimate the sources and types errors in chemical analysis.
4	Explain the terms such as mean, median, precision, accuracy, absolute error and relative error and interpret the effects of systematic errors on analytical results.
5	Explain the terms such as standard solution, titration, back titration, equivalence point, end point, primary and secondary standard and can carry out the calculations
6	Select suitable gravimetric analysis method for determining the quantity of the substance.
7	Describe the properties of precipitate and precipitating agents.
8	Define electromagnetic spectrum and establish relation between frequency, wavelength, wave number and the energy aspects.

9	Explain spectrophotometric methods of determination of various metal ions
10	Describe and differentiate different types of scattering along with applications of turbidimetry and nephelometry.
11	Explain different separation methods employed in analytical chemistry.
12	Compare the efficacy of solvent extraction and chromatographic methods for adopting suitable method for separation.
13	Describe TGA, DTA and DSC, their principles and applications.

Course: Computational Chemistry	**Course Code:** 21 ICH1 S1 LP
Teaching Hours/Week (L-T-P):1 - 0 - 2	**No. of Credits:** 02
Internal Assessment: 20 Marks	**Semester End Examination:** 30 Marks

Course Objectives:

1. The goal of this course is to cover the fundamental mathematical approaches utilised by chemists in industries.

Unit 1: Introduction to Mathematics for Chemists with MATLAB

Theory

1. Chemists in Industries - An intro to what computational skills are relevant in industries
2. Introduction to Vectors and Matrix calculations
3. Introduction to Calculus for Chemists

Practical

1. Introduction to MATLAB – Matrix calculations with MATLAB
2. Symbolic Calculus using MATLAB
3. Symbolic Integration and Differentiation
4. Data Analysis using MATLAB (Working with Potentiometric Data)

Unit 2: Analysis of Chemical Reaction Kinetics

Theory

1. Analysis on effects of process parameters on Chemical Kinetics
2. Introduction to adsorption- Equilibrium models, BET Surface area analysis
3. Reaction kinetics with heterogeneous catalysis

Practical

1. Analysis of fundamental chemical kinetics-1st, 2nd and 3rdorder reactions
2. Effect of feed concentration ratio and temperature on yield of series parallel reactions
3. Computing adsorption isotherm from experimental data
4. Calculating the adsorbent BET surface area from adsorption-desorption data
5. Case study: Effect of rate of adsorption and rate of surface reaction on overall reaction rate in heterogeneous catalysis

Course Outcomes: After completing this course, students will be able to

CO	Statement
1	Address complex issues in chemical kinetics adsorption, material characteristics, and so on.
2	Use industry standard computational tools

Course: Inorganic Chemistry Practicals	**Course Code:** 21 ICH1 C1 P
Teaching Hours/Week (L-T-P): 0 - 0 - 4	**No. of Credits:** 02
Internal Assessment: 20 Marks	**Semester End Examination:** 30 Marks

Course Objectives:

1.The objective of this course is to make the students to understand and perform both qualitative and quantitative analytical techniques for detection and determination.

List of Experiments

1. Semi-micro qualitative Analysis:

Semi-micro qualitative Analysis of Inorganic mixture containing 2 anions (one interfering anion) and 2 cations (one rare cation). Minimum number of mixtures to be analysed - 5

2.Quantitative Inorganic Analysis: Titrimetry

i) Determination of calcium using $KMnO_4$

ii) Determination of copper using KIO_3

iii) Determination of Iron using ceric ammonium sulphate

iv) Determination of Aluminium using EDTA

3. Quantitative Inorganic Analysis: Gravimetry

i) Determination of sulphate as Barium sulphate.

ii) Determination of Nickel as NiDMG.

References:

1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J.Mendham, ELBS (1986).
2. Vogel's text book of Quantitative Chemical Analysis, 5th Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical (1999).
3. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co.(1974).
4. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co.,London (1972).

Course Outcomes (CO): After the completion of this course, the student would be able to ;

CO	Statement
1	Explain the systematic methodology used in qualitative analysis of inorganic substances and implement the same wherever required.
2	Carryout the preparation of standard solutions accurately to minimise errors.
3	Enhance the skill to do titrations and identify the end point accurately.
4	Determine the quantity of unknown substances accurately.

Course: Organic Chemistry Practical's	**Course Code:** 21 ICH1 C2 P
Teaching Hours/Week (L-T-P): 0- 0 - 4	**No. of Credits:** 02
Internal Assessment: 20 Marks	**Semester End Examination:** 30 Marks

Course Objectives:
1.The objective of this course is to make the students to understand and perform quantitative analysis of different organic compounds

List of Experiments

Quantitative analysis
1. Titrimetric estimation of amino acids.
2. Saponification value of oil.
3. Estimation of glucose by Fehling's method.
4. Estimation of keto group.
5. Estimation of phenols.
6. Iodine value of oil (chloramine-T method).

Qualitative analysis
Systematic analysis and identification of organic compounds

References:

1. Laboratory manual of Organic Chemistry- B. B. Dey, M V Sitaraman and T RGovindachari, Allied Publishers, New Delhi, (1996).
2. Practical Organic Chemistry – Mann and Saunders, (1980).
3. Text Book of Practical Organic Chemistry- A. I. Vogel, (1996).
4. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
5. A Handbook of Organic Analysis – Clarke and Hayes, (1964).
6. Comprehensive practical organic chemistry: Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
7. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S.Dhingra, Universities Press (India), 2000.
8. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
9. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
10. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.

Course Outcomes (CO): After the completion of this course, the student would be able to;

CO	Statement
1	Analyse amino acid content in different pharmaceutical samples
2	Estimate saponification and iodine values of oil samples.
3	Determine phenol content in different samples.
4	Find out glucose content in a given sample.

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Course: Analytical Chemistry Practical's	**Course Code:** 21 ICH1 C3 P
Teaching Hours/Week (L-T-P): 0 - 2 - 0	**No. of Credits:** 02
Internal Assessment: 20 Marks	**Semester End Examination:** 30 Marks

Course Objectives:

1.In the first semester laboratory, students will gain the hands on skill of handling the PH meter, potentiometer, skill on preparation of solutions with known concentrations. conductometer. complementary to the learning objective of discipline specific course, student should carry out the experiments related to determination of rate constants, energy of activation and adsorption phenomenon

List of Experiments

1.Determination of molal boiling point elevation constant of water using (1) NaCl (2) Urea and (3) Oxalic acid as solutes
2. pH titration of HCl with NaOH
3. Determination of Equivalent Conductance at infinite dilution of a strong electrolyte
4. Determination of pKa1 and pKa2 of Oxalic acid by PH titration
5. Conductometric titration of a mixture of strong and weak acid with strong base
6.Estimation of Iron using Potassium dichromate by potentiometric titration
7. Kinetics of hydrolysis of ester using HCl and H2SO4 at two different temperatures and determination of rate constants and energy of activation
8.Study of kinetic reactions between K2S2O8 and KI determination of rate constants and energy of activation
9.Conductometric titration of a mixture of H2SO4, acetic acid and cupper sulphate penta hydrate using a strong base
10.Phase diagram of three component system. Acetic acid, Benzene and water
11. Adsorption of acetic acid on Charcoal
12. Adsorption of oxalic acid on charcoal

References:

1. Findlays Practical physical chemisty revised by P. B. Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966)
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988)
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987)
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968)
7. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, NewYork (1962)
8. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi(1983)
9. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International,New York (2001)
10. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow,
S. R. Cohen and M. E. Green Macmillan publishing Co .New York.
11. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers Delhi (2006).

Course Outcomes (CO): At the end of the practical physical chemistry course, student should acquire a skill to;

CO	Statement
1	1. Read properly end points in titrations.
2	Plot the graphs of potentiometric behaviour of redox titration
3	Reproduce the value of rate constants
4	Predict the energy of activation
5	Verify the Raoults law on colligative properties
6	Observe the change in the PH and conductance behaviour of the reaction
7	Construct the phase diagram of three component system
8	Describe the adsorption phenomenon

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