TECHNO INDIA UNIVERSITY
WESTBENGAL

EM 4, Sector V, Salt Lake, Kolkata-700091, West Bengal, India
Phone: +91 9836544416/17/18/19, Fax: +91 33 2357 1097

2-Year Master of Science (M.Sc.) Curriculum and Syllabus for Chemistry

Second Semester

Course Code	Course Title	Contact Hrs. / Week			Credit
		L	T	P	
Theory					
TIU-PEN-T100	Career Advancement Skill Development	2	1	0	3
TIU-PCH-T102	Physical Chemistry	3	1	0	3
TIU-PCH-T104	Organic Chemistry	3	1	0	3
TIU-PCH-T106	Inorganic Chemistry	3	1	0	3
TIU-PCH-T108	Analytical Chemistry	3	1	0	3
Practical					
TIU-PCH-L104	Organic Chemistry Lab	0	0	3	2
TIU-PPH-L114	Computer Application in Chemistry	1	0	3	3
Sessional					
TIU-PES-S198	Entrepreneurship Skill Development	0	0	2	2
	Total	15	5	6	**22**

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Semester-II

Physical Chemistry
TIU-PCH-T102

L-T-P: 3-1-0 **Credit: 3**

Module 1

Electrochemistry

Quantitative treatment of Debye-Hückel theory of ion-ion interaction and activity coefficient, applicability and limitations of Debye-Hückel limiting law, its modification for finite-sized ions, effect of ion-solvent interaction on activity coefficient. Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution, its applicability and limitations, Pair-wise association of ions (Bjerrum and Fuoss treatment), Modification of D-H-O theory to account for ion-pair formation, Determination of association constant (K_A) from conductance data.

Module 2

Surface Chemistry

A. Reactions on surfaces: Adsorption, adsorption isotherms, unimolecular surface reaction, bimolecular surface reactions-reaction between a gas molecule and an adsorbed molecule, reaction between two adsorbed molecules, inhibition and activation energy of such reactions, volcano curve.

B. Transition state theory of surface reactions: rates of chemisorptions and desorption, unimolecular and bimolecular surface reaction, comparison of homogeneous and heterogeneous reaction rates.

C. Micelles: Surface active agents and their classifications, micellization, factors affecting cmc of surfactants, Thermodynamics of micellization: phase separation and mass action models, micro-emulsions, reverse micelles.

Module 3

Quantum Mechanics

A. Fundamentals of quantum mechanics: Black-body radiation, photoelectric effect, Davison and Germer experiment, Franck-Hertz experiment, Young's double slit experiment; identification of classical and quantum systems, Bohr's correspondence principle with examples, the uncertainty principle.

B. Operators in quantum mechanics: Eigenvalues and eigenfunctions, Hermitian operator and its application. Postulates of quantum mechanics, Angular momentum of a one-particle system, and its commutative relations, Ladder operator, Pauli spin operator, Pauli spin matrices-spin

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eigenfunctions and their properties, Schrodinger wave equation and its formulation as an eigenvalue problem.

C. Quantum mechanical treatment on various systems: Translational motion of a particle, particle in one and three dimensional boxes, harmonic-oscillator, rotational motion of a particle: particle on a ring, particle on a sphere, rigid rotator, step-potential and tunneling, hydrogen atom.

D. Approximation methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples, Variation method.

Books Recommended

1. J. O'M. Bockris, A. K. N. Reddy, Modern Electrochemistry, Vol. 2 A & B, 2nd Edition, Plenum Press, New York (1998).
2. Samuel Glasstone, An Introduction To Electrochemistry, Affiliated East-West Press Pvt. Ltd.- New Delhi (2000)
3. A. J. Bard, L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications; 2nd Edition (2001), John Wiley & Sons, New York.
4. Y. Moroi, Micelles: Theoretical and Applied Aspects, Plenum Press, New York (1992).
5. P. W. Atkins, Physical Chemistry, 7th & 8th Editions, Oxford University Press, New York
6. I. N. Levine, Quantum Chemistry, 5th Edition (2000), Pearson Educ., Inc. New Delhi.
7. D. A. McQuarrie, J. D. Simon, Physical Chemistry, A Molecular Approach, (1998), Viva Books, New Delhi.

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Organic Chemistry
TIU-PCH-T104

L-T-P: 3-1-0 **Credit: 3**

Module 1

Pericyclic reactions: Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-buta diene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach, concept of aromaticity of pericyclic transition states. Selection rules and stereochemical aspects of electrocyclic reactions, cycloaddition and sigmatropic shifts. Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Sommelet-Hauser, Cope, Claisen, and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Module 2

Esterification and hydrolysis of ester: Evidence for tetrahedral intermediate in BAc2 and AAc2 mechanisms, steric and electronic effects, the AAc1 and other pathways involving alkyl to oxygen bond cleavage.

Module 3

A. Electrophilic and nucleophilic aromatic substitution: Electrophilic aromatic substitution: The Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/para ratio, Ipso substitution. Nucleophilic aromatic substitution: The Aromatic S_N1, S_N2 and benzyne mechanisms. Reactivity-effect of substrate structure, leaving group, and attacking nucleophiles.

B. Elimination reaction mechanism: The E1, E2, and E1cB mechanisms, Orientation of double bond, Hoffman elimination, Saytzeff elimination, Hoffman versus Saytzeff elimination, Pyrolytic-*syn*-elimination, competition between substitution and elimination reactions.

Module 4

Formation and reactions of enol and enolate: Enol and enolate, Stable enol, consequence of enolization, Reactions with enols and enolates as intermediate, Stable enolate ions, Preparation of enol ether, Reactions of enol ethers.

Books recommended

1. Clayden, Greeves, Warren, Wothers, Organic Chemistry, Oxford University Press, 2001.
2. M. B. Smith, Jerry March, Advanced Organic Chemistry, 5th Edition (2001), John Wiley & Sons, New York.
3. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th Edition (1997), Orient

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Longman Ltd., New Delhi.
4. G. S. Zweifel, M. H. Nantz, Modern Organic Synthesis, (2007), Freeman and Company, New York.
5. S. M. Mukherjee, S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition (1990), Macmillan India Ltd., New Delhi.
6. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition).
7. S. M. Mukherjee, S. P. Singh, Pericyclic Reactions, MacMillan India, New Delhi.
8. I. Fleming, Pericyclic Reactions, Oxford University Press, Oxford (1999).

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Inorganic Chemistry
TIU-PCH-T106

L-T-P: 3-1-0 **Credit: 3**

Module 1

A. Kinetics and Mechanism of Substitution Reactions: Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral and square-planar complexes in terms of crystal field activation energy and structure preference energy; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.

B. Electron Transfer Reactions: Mechanism and rate laws; various types of electron transfer reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions; identification of intervalence transfer bands in solution.

Module 2

Metal Carbonyls and related compounds: Preparation, structure, and properties: bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls, principal reaction types of metal carbonyls.

Module 3

Chemistry of Lanthanides and Actinides: Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex- chemistry, electronic spectra and magnetic properties, lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides, organo-lanthanoids and actinoids.

Books Recommended

1. F. Basalo, R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Edn. (1967), Wiley Eastern Ltd., New Delhi.
2. D. F. Shriver, P. W. Atkins, Inorganic Chemistry, 3rd Edn. (1999), ELBS, London.
3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 6th Edn. (1999), John Wiley & Sons, New York.
4. D. N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, Universities Press (India) Ltd., Hyderabad (2001).
5. Keith F. Purcell, John C. Kotz, Inorganic Chemistry, W. B. Saunders Com. (1987), Hong Kong.
6. Martin L. Tobe, John Burgess, Inorganic Reaction Mechanisms, Longmans 1st Edn. (1999).

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Analytical Chemistry
TIU-PCH-T108

L-T-P: 3-1-0 **Credit: 3**

Module 1
Spectroscopic Techniques
Theory, Instrumentation and applications of Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry, UV-Visible molecular absorption Spectrometry (principles, instrumentation, and application), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence), Concept of Inductively coupled plasma-atomic absorption spectrophotometer, ICPA-AAS (Instrumentation and application).

Module 2
Chemical Sensors and Separation Techniques
A. Principles, types of chemical sensors based on the modes of transductions, Types of chemical sensor based on the chemically sensitive materials (solid electrolyte, gas, semiconductor), Humidity sensors, Biosensors, Electrochemical sensors (Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

B. Principles of chromatography, Classification of chromatography, Paper chromatography, Techniques of Column chromatography, Thin layer chromatography, Gas Chromatography, High-performance liquid chromatography, Ion chromatography.

Module 3
Voltammetry and Thermal Analysis
Linear sweep voltammetry, Anode sweep voltammetry, Cyclic voltammetry, Polarography, Current-Voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, ilkovic equation (derivation excluded), Differential pulse polarography, Qualitative and Quantitative applications. Thermal Analysis: Theory, methodology and application of Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry (DSC). Principles, techniques, and application of thermometric titration methods, Amperometric titrations.

Recommended books

1. D.A. Skoog, Principles of Instrumental Analysis, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.
2. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Analytical Chemistry-An Introduction, 7th Edition, (2000), Saunders College Publishing, Philadelphia, London.
3. Nirmalendu Nath, Kakoli Upadhyay, Avinash Upadhyay, Biophysical Chemistry Principles and Techniques, Himalaya Publishing house, New Delhi.
4. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.

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5. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5th Edition (1978), McGraw Hill Books Co, New York.
6. Modern method of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
7. G.D. Christian,, R. L. Pecsok, L. D. Shields, T. Cairns, L.C. Mc William, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.

Computer Application in Chemistry
TIU-PPH-L114

L-T-P: 1-0-3 **Credit: 3**

Module 1
Programming in C
Decision making, looping, and control structures. Functions; recursion; arrays; introduction to pointers; character strings; structures and unions, managing input/output operations, formatted I/O, standard library/user-defined functions.

Module 2
Numerical Methods
Approximations and round off errors, Truncation errors, Determination of roots of polynomials and transcendental equations by Newton-Raphson, Secant and Bisection's method.
Backward, Forward, Newton-Divided Difference Ploynominal, integration.

Module 3
Applications of MATLAB in Chemistry
Solving ordinary and partial differential equations using MATLAB. Solver methods for stiff and non-stiff ordinary differential equations. Finite element analysis. Applications in statistical mechanics and chemical thermodynamics, Bayesian statistics, stocastic simmulation and parameter estimation. Monte-Carlo simulation. Statistical inference. Time series analysis and ANOVA.

Recommended Books

I. Programming in C
1. Let Us C, Yashwant Kanetkar
2. Programming in ANSI - C, Balagurusamy, E, Tata McGraw-Hill
II. Numerical Methods

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3. Numerical Analysis, S. Ali Mollah
4. Introductory Numerical Analysis, Dutta & Jana

III. Applications of MATLAB in Chemistry

5. K. J Beers, Numerical Methods for Chemical Engineering: Applications in MATLAB, Cambridge University Press, 2007.

Organic Chemistry Lab
TIU-PCH-L104

L-T-P: 0-0-3 **Credit: 2**

Experiment 1: Characterization of organic compounds or groups by spectroscopic methods

Experiment 2: Separation of aromatic compounds utilizing their physical properties

Experiment 3: Isolation of caffeine from tea leaves

Experiment 4: Separation, and identification of organic compounds in binary mixtures

Experiment 5: Separation and identification of organic mixtures containing up to three components.

Experiment 6: Preparation of organic compounds involving several stages, characterization of intermediates and final products by IR and NMR spectroscopy.

Experiment 7: Techniques of organic chemistry: Special practical's involving steam distillation, photo-isomerisation and thin layer chromatography etc.

Experiment 8: Quantitative analysis of (i) sulfur and (ii) nitrogen.