Rayat Shikshan Sanstha's

YASHAVANTRAO CHAVAN INSTITUTE OF SCIENCE, SATARA

(An Autonomous College)

Reaccredited by NAAC with 'A+' Grade

New Syllabus For

Master of Science

Part - II

Physical Chemistry

Syllabus

to be implemented from June, 2022 onward

Structure of the course

M.Sc. Part II Semester III

Theory			
Course No. and Course code	**Title of Course**	**No. of lectures Per week**	**Credits**
MPCT-301	Advanced Quantum Chemistry	4	4
MPCT-302	Electrochemistry	4	4
MPCT-303	Molecular Structure - I	4	4
Elective Course			
MPCT-304A or MPCT-304B	Applied Physical Chemistry or Radiation and Photochemistry	4	4
Practical			
MPCP 305	Practical course V: Lab V	16	4
MPCP 306	Practical course VI: Lab VI	16	4
		48	24

M.Sc. Part II Semester IV

Theory			
Course No. and Course code	**Title of Course**	**No. of lectures Per week**	**Credits**
MPCT-401	Thermodynamics and molecular modelling	4	4
MPCT-402	Chemical Kinetics	4	4
MPCT-403	Molecular Structure - II	4	4
Elective Course			
MPCT-404A or MPCT-404B	Physicochemical Techniques or Surface Chemistry	4	4
Practical			
MPCP 405	Practical course V: Lab VII	16	4
MPCP 406	Practical course VI: Lab VIII	16	4
		48	24

M. Sc. II Evaluation Pattern

Paper code	Theory			Practical			Total
	ESE	ISE	Total	ESE	ISE	Total	
Theory paper - I	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Book review) Total = 40	100	--	--	--	100
Theory paper - II	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Home assignment) Total = 40	100	--		--	100
Theory Paper - III	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Survey/Seminar) Total = 40	100	--	--	--	100
Theory paper - IV	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Group discussion / Innovative idea presentation) Total = 40	100	--	--	--	100
Practical paper - I	--	--	--	60	Journal = 10 Student performance = 10 Activity = 20 (case study/survey report) Total = 40	100	100
Practical paper - II	--	--	--	60	Journal = 10 Student performance = 10 Activity = 20 (model presentation/project) Total = 40	100	100
Total	**240**	**160**	**400**	**120**	**80**	**200**	**600**

M. Sc. Part-II (Semester III)

MPCT 301: Advanced Quantum Chemistry

Course Objectives: Student will be able to

1. understand basic concepts in quantum chemistry.
2. understand the variation principle and Hückel Molecular Orbital Theory.
3. learn the theoretical Ab initio methods.
4. comparative study of various semi-empirical methods.

Credits = 4	**SEMESTER-III** **MPCT 301: ADVANCED QUANTUM CHEMISTRY**	**No. of hours per unit/ credits**
UNIT I	**Basics of Quantum Chemistry**	**(15)**
	Brief review of basic principles of quantum mechanics. Operators in quantum mechanics. Exact solution of Schrödinger wave equation for rigid rotator, linear harmonic oscillator and hydrogen and hydrogen like atoms. Transition dipole moment integral and selection rules for rotational, vibrational and electronic transitions.	
UNIT II	**Variation Principle and Hückel Molecular Orbital Theory**	**(15)**
	Variation principle and its application to some simple systems. Hückel molecular orbital theory – Assumptions of HMO theory, Paulis exclusion principle, quantum number, the Born-Oppenheimer approximation, -electron approximation, Secular determinant and secular equations, Hückel rule and aromaticity, HMO calculations for organic molecules, free valence index and prediction of chemical reactivity, use of molecular symmetry for simplification of HMO calculations, HMO treatment for molecules containing heteroatoms, extended Hückel methods.	
UNIT III	**Ab initio methods**	**(15)**
	Self-consistent field (SCF) theory, Hartree-Fock (HF) method, quantum particles and their spins, properties of slater determinant, HF equation, restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock (UHF) models, Fock matrix, HF calculations, Roothan-Hall equations, Koopman's theorem, electron correlation method. Basis sets: Slater type orbitals (STO), Gaussian type orbitals (GTO), difference between STO and GTO, energy calculations using such orbitals for multielectron	

	systems, classification of basis sets, minimal basis sets, energy calculations for H-atom using STO basis sets at different levels, double- and triple-zeta basis sets, valence-split basis sets, polarized basis sets, truncation and superposition errors in basis sets, methods to overcome above errors. Correlation energy, configuration interactions, many body perturbation theory, Möller-Plesset perturbation, coupled cluster method. Introduction to various software packages for performing ab initio and density functional theory calculations.	
UNIT IV	**Semi-empirical methods and Molecular Mechanics, Semi-empirical Methods**	**(15)**
	Introduction, need of semi-empirical methods, zero differential overlap (ZDO) approximation, neglect of differential overlap (NDO) method, complete neglect of differential overlap (CNDO), intermediate neglect of differential overlap (INDO), modified intermediate neglect of differential overlap (MINDO), modified neglect of differential overlap (MNDO), neglect of diatomic differential overlap (NDDO). AM1, PM3, PM5, PM6 etc. methods, Chemical Hamiltonian approach, Hamiltonian in semi-empirical methods, comparisons in various above-mentioned methods, limitations of semi-empirical methods. Introduction to various software packages for performing semi-empirical calculations.	

Course Outcomes: Student should be able to

1. derive Shrodinger wave equation.
2. explain the exact concept of Huckel molecular orbital theory as well as variation principle.
3. calculate various parameters based on ab Initio method and DFT.
4. compare the semi-empirical methods and ab-initio methods.

References: -

1) A. K. Chandra, Introductory Quantum Chemistry, (Tata McGraw- Hill, New), 4th edition, 1994. (Unit I, II)

2) P. Atkins and R. Friedman, Molecular Quantum Mechanics, (Oxford University Press, New York) 4th Edition, 2005. (Unit IV)

3) Ira N. Levine, Quantum Chemistry, (Pearson, City University of New York), 7th edition, 2019. (Unit I)

4) R. K. Prasad, Quantum Chemistry (New Age International (P) Limited Publishers), 1997. (I, II, III, IV)

MPCT 302: ELECTROCHEMISTRY

Course Objectives: Student will be able to

1. understand electrokinetic phenomena of solutions.
2. study the ion-solvent interaction in details.
3. learn the exact meaning of electrode reactions in electronic devices.
4. understand the significance of fuel cells and concept of corrosion.

Credits = 4	**SEMESTER-III** **MPCT 302: ELECTROCHEMISTRY**	**No. of hours per unit/ credits**
UNIT I	**Electrokinetic phenomena**	**(15)**
	Electrical double lever, stern theory of the double layer, electro-capillary phenomena, electro-capillary curve. electro-osmosis, electrophoreses. Streaming and Sedimentation potentials. Zeta potentials and its determination by electrophoresis, influence of ions on Zeta potential.	
UNIT II	**Ion-solvent Interactions**	**(15)**
	Structure of water, hydration, heats of hydration of electrolytes, individual ions and their comparison, calculation of heats of hydration (Born, Van Arkel & de Boer, Bernal-Fowler methods), entropy of hydration and hydration numbers. Ion transport in solutions, diffusion, chemical potential and work of transport, Ficks laws, expressions for flux and diffusion coefficient. Ionic liquids: Introduction, difference between electrolytes and ionic liquids, diffusionin fused salts, viscosity and diffusion coefficient in molten salts.	
UNIT III	**Electrode reactions**	**(15)**
	Electrified interface, electron transfer under interfacial electric field, symmetry factor, electrode at equilibrium, exchange current density, over potential, Butler-Volmer equation, high field and low field approximations, Tafel equations, kinetics of discharge of hydrogen ions. Diffusion over potentials. Electrode kinetics of semiconductor/ solution interface; n and p type semiconductor, current-potential relation of n and p type semiconductors.	

UNIT IV	**Fuel cells and corrosion**	**(15)**
	Significance of fuel cells: hydrogen - oxygen, hydrocarbon - air, PAFC (Phosphoric acid Fuel cell), Proton exchange membrane fuel cell, solid oxide fuel cell and alkaline fuel cell **Corrosion**: concept and importance, mechanism of corrosion and Pourbaix.	

Course Outcome: Student should able to

1) explain electrokinetic phenomena useful in electrochemistry.
2) clarify the ion-solvent interactions in electrochemistry.
3) decide those the electrode reactions useful to the development of energy devices.
4) explain the reaction involving in fuel cells as well as corrosion in electrochemistry.

REFERENCE BOOKS:

1) S. Glasstone, An Introduction to Electrochemistry, (East West Press Private Limited.), 1942. (Unit I)
2) J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, (Kluwer Academic Publishers,New York,) Vol. I & II 2000. (Unit II)
3) S. Glasstone, Text book of Physical Chemistry, (Frink chemical laboratory, Princeton University), 1940. (Unit II)
4) R. A. Robinson and R. H. Strokes, Electrolytic Solutions, 1959. (Unit I)
5) Fuel cell systems explained 2nd ed. by games larminie Andrew Dicks, Jahn wiley & sons Ltd., Atnum, southern gate, west Sussex PO1985 Q (England). (Unit IV)

MPCT 303: MOLECULAR STRUCTURE - I

Course Objectives: Student will be able to

1. learn the symmetry of different inorganic and organic molecules.
2. understand the fluorescence spectroscopy in details.
3. study about the IR and Raman spectroscopy.
4. study electronic spectroscopy for analysis of electronic spectra of polyatomic molecules.

Credits = 4	**SEMESTER-III** **MPCT 303: MOLECULAR STRUCTURE - I**	**No. of hours per unit/ credits**
UNIT I	**Symmetry properties of molecules and group theory**	**(15)**
	Symmetry elements, symmetry operations and point groups, properties of group, symmetry operations as a group, multiplication table. Classes of symmetry operations, basis, representative and matrix representations of operations. Reducible and irreducible representations, orthogonality theorem. Properties of irreducible representations. Constructions of character table for point groups. Explanations for the complete character table for a point group. Representations of vibrational modes in nonlinear molecules. Infrared and Raman activities of normal modes of vibrations.	
UNIT II	**Fluorescence spectroscopy**	**(15)**
	Photoluminescence, instrumentation, electronic transition in atoms and molecules, solvatochromism, rate of excited molecules, structural factors, properties of fluorescence, Fluorescence parameters: fluorescence intensity, quantum yield and fluorescence life time, corrected emission and excitation spectrum, relation between emission spectrum and excitation spectrum, inner filter effect, solvent effect of fluorescence, solvation dynamics, effect of intermolecular process, relation between concentration with fluorescence and phosphorescence intensity, fluorescence quenching, energy transfer, excited state proton transfer, synchronous spectrum, fluorescent nanomaterials and its applications.	
UNIT III	**Infrared spectroscopy and Raman Spectroscopy**	**(15)**
	Diatomic molecules: Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero-point energy, isotope effect. The anharmonic oscillator, the diatomic vibrating rotator, the interactions of rotations and vibrations. Polyatomic molecules: Fundamental vibrations and their symmetry, overtone and combination frequencies. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Analysis by Infrared techniques. Raman Spectroscopy: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman	

	Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Polarization of light and the Raman effect. Structure determination from Raman and Infrared spectroscopy. Techniques to simple structural problems.	
UNIT IV	**Electronic Spectroscopy**	**(15)**
	General nature of band spectra. Beer- Lambert law integrated absorption coefficient and oscillator strength. Term symbols for atoms and molecules. The hydrogen atom and hydrogen like species spectrum. Sequences and progressions, the vibrational course structure and rotational fine structure of electronic band. The Franck-Condon principle, dissociation energy and dissociation products. Birje-Sponer extrapolation.The fortrat diagram. Predissociation, classification of electronic states. The spectrum of molecular hydrogen. Electronic spectra of polyatomic molecules. Chemical analysis by electronic spectroscopy. (d-d), (CT) and (n-π*) transitions. Photochemical mechanism of vision.	

Course Outcomes: Student should be able to

1. calculate elements of symmetry for all molecules.
2. explain fluorescence spectroscopy in details.
3. compare the infrared spectroscopy and raman spectroscopy in details.
4. analyze electronic spectra of polyatomic molecules.

References: -

1) R. K. Prasad, (New Age International (P) Limited Publishers), 2006. [Unit I]
2) C. N. Banwell, Fundamental of molecular spectroscopy, (McGraw-Hill Book Co. (U. K. Ltd), 3rd Edition, 1983. (Unit III, IV)
3) P. W. Atkins, Physical Chemistry, (Freeman: New York), 1976. (Unit I)
4) I. N. Levine, Molecular Spectroscopy, (New York: Wiley), 1975. (Unit III, IV)
5) G. M. Barrow, Molecular Spectroscopy, (McGraw-Hill Book Co. New York, USA), 1962. (Unit III, IV)
6) K. K. Rohatgi-Mukherjee, Fundamentals of photochemistry (New Age International publisher), 3rd Edition, 2014. (Unit II)

Additional reading

7) D. L. Pavia, G. M. Lopmann G. S. Kriz, Introduction spectroscopy, (Brooks/Cole Cengage Learning), 4th Edition, 2006. (Unit III, IV)
8) K. Veera Reddy, Symmetry & spectroscopy of molecules, (New Age International publisher), 2nd revised Edn., 2009. [Unit I]

Elective Course

MPCT 304 A: Applied Physical Chemistry

Course Objectives: Student will be able to

1. study the methods of X-ray structure analysis of crystals.
2. understand the different types of solid-state reactions and crystal defects.
3. study the electronic properties of semiconductors.
4. understand the role of heterogeneous catalysis in recent research.

Credits = 4	**SEMESTER-III** **MPCT 304 A: Applied Physical Chemistry**	**No. of hours per unit/ credits**
UNIT I	**The solid state**	**(15)**
	Introduction, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Miller indices, Bragg Method, Debye-Sherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-Ray intensities, structure factor and its relation to intensity and electron density, phase problem, procedure for an X-ray structure determination.	
UNIT II	**Solid State Reactions and crystal defects**	**(15)**
	A) Solid State Reactions General principle, types of reactions: Additive, structure sensitive, Decomposition and phase transition reactions, tarnish reactions, kinetics of solid-state reactions, factors affecting the reactivity of solid-state reactions. **B) Crystal defect** Classification of defects subatomic, atomic & lattice defects in solid	
UNIT III	**Electronic Properties and Band Theory**	**(15)**
	Metals, insulators and semi conductors, free electron theory and its applications, electronic structure of solids, band theory, band structure of metals, insulator, and semiconductors, doping in semiconductors, p- n junction, superconductors, molecular materials, organic materials, some examples of organic semiconductors, charge carrier injection and transport, optical properties of organic semiconductors, applications and devices involving optical properties,	

	luminescence photoluminescence, effect of impurity levels on photoluminescence, light emitting diodes, luminous efficiency, photo-conduction and photoelectric effects, laser, principle of laser action, solid state laser and their applications.	
UNIT IV	**Catalysis**	**(15)**
	i) Fundamentals of adsorption and catalysis: Physical and Chemical adsorption–adsorption isotherms: evaluation, chemisorption on metals and metal oxides. Catalysis: concept of activity, selectivity, poisoning, promotion and deactivation. Types of catalysis: homogeneous, heterogeneous. Heterogeneous catalysis and catalytic kinetics: concept of Langmuir-Hinshelwood **(5L)** ii) Preparation and Characterization of Catalyst: general methods for preparation of catalysts: precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation of catalysts: calcinations, reduction. Catalyst characterization: surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FT-IR and thermal methods. **(5L)** iii) Nanomaterials and Catalysis: General definition, Nanochemistry basics, distinction between molecules, nanoparticles and bulk materials. Physicochemical considerations of nanomaterials. Size-dependent properties. **(3L)** iv) Photo-catalysis: Photoprocesses at metals, oxides and semiconductors: concepts and mechanism. Photocatalysis application in organic pollutant degradation present in water and air. **(2L)**	

Course Outcomes: Student should be able to

1. analyse crystal structure of cubic systems.
2. describe various types of solid-state reactions and crystal defects.
3. select semiconductors based on their electronic properties that are useful in optoelectronic devices.
4. explain how nanomaterials as well as heterogeneous catalysis play a significant role in current research.

References: -

1) J. N. Gurtu, Solid state chemistry (Pragati Prakashan), 1st edition 2012. [Unit I, II]
2) A. R. west(plenum), Solid state chemistry and its applications, (John Wiley & Sons), 1984. [Unit I, II]
3) Gerald R. Van Hecke & Kerry K. Karukstis, A Guide To lasers in chemistry, (Boston, Mass.: Jones and Bartlett), 1998. [Unit III]
4) W. Adamson, Physical Chemistry of Surfaces, (Wiley Intersciences), 5th edition 1990. [Unit IV]
5) 5) G. C. Bond, Heterogeneous Catalysis: Principles and Application, (Oxford University Press),1987. [Unit IV]
6) D. K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, (New Age International Publishers) Oct 2008. [Unit IV]
7) B. C. Gates, Catalytic Chemistry, (John Wiley and Sons Inc.), 1992. [Unit IV]
8) G. Cao, Nanostructures and Nanomaterials - Synthesis, Properties and Applications, World- Scientific, (Imperial College Press), 2004. [Unit IV]

MPCT 304-B: Radiation and Photochemistry

Course Objectives: Student will be able to

1. study the various types of radiation and their uses in chemical processes.
2. understand the laser induced chemical reactions.
3. know the basics concept of photochemical devices.
4. learn about the various types of photochemical reactions.

Credits = 4	**SEMESTER-III** **MPCT 304-B: Radiation and Photochemistry**	**No. of hours per unit/ credits**
UNIT I	**Radiation Chemistry**	**(15)**
	Introduction, Radiation Types, their characteristics, Radiation in chemical processes.	
UNIT II	**Lasers and Lasers in Chemistry**	**(15)**
	Introduction, characteristics of laser, uses of lasers in chemical process, laser induced chemical reactions, organic photochemistry, lasers as a photochemical tool, laser induced selective bond chemistry, overview, bond selective chemistry of light atom molecules.	
UNIT III	**Basics of photochemistry**	**(15)**

	Electrochemistry of excited states, life time measurements, flash photolysis, energy dissipation by radiative and non-radiative processes, properties of excited states, structure, dipole moment, acid-base strength, reactivity, photochemical kinetics, calculations of rates of radiative process, bimolecular quenching, Luminescence for sensors and switches, charge transfer excited state, photoinduced electron transfer reactions.	
UNIT IV	**Miscellaneous Photochemical reaction**	**(15)**
	Photo-fries reaction of anilides, photo - fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog, photodegradation of polymers, photochemistry of vision.	

Course Outcomes: Student should be able to

1) determine which types of radiation are used in chemical processes.
2) explain how radiation plays an important role in chemical reactions.
3) learn the energy dissipation by radiative in photochemical devices.
4) explain the role of light on chemical reactions of light atom molecules.

References: -

1) N. J. Turro, W. A. Benjamin, Molecular Photochemistry Inc., New York-Amsterdam, 1965. [Unit I, IV]
2) K. K. Rohatagi - Mukherji, Fundaments of Photochemistry, (Wiley -Eastern New Delhi), 1978. [Unit II]
3) G. S. Ferraudi, Elements of Inorganic Photochemistry, (New York: J. Wiley), 1988. [Unit III]
4) A. W. Adamson & P. J. Fleischauer, Concepts of Inorganic Photochemistry, (Wiley, New York), 1975. [Unit III]
5) Gerald R. Van Hecke & Kerry K. Karukstis. A Guide To lasers in chemistry, (Boston, Mass.: Jones and Bartlett), 1998. [Unit II]

MPCP-305 Physical Chemistry Practical Course-V (Lab-V)

Course Objectives: Student will be able to

1) know and understand the instrumental analysis
2) learn about determining thermodynamic parameters for electrochemical reactions.
3) study the determination of crystal structure of simple cubic system.
4) understand order of reactions and half wave potential of reactions.

Credits=4	**SEMESTER-III** **MPCP-305 Physical Chemistry Practical Course-V (Lab-V)**	**No. of hours per unit/ Credits (60)**
I	**Spectroscopy and chemical kinetics**	
	1) Spectrophotometry To determine pK value of methyl red indicator at room temperature spectrophotometrically. **2) Amperometry** To determine unknown concentration of Iodine using amperometry **3) Chemical Kinetics** To determine the order of reaction between acetone and iodine catalyzed by acid.	
II	**Potentiometry, conductometry and XRD analysis**	
	1) Potentiometry To determine instability constant and stoichiometry of silver ammonia complex potentimetrically. **2) Conductometry** Determination of the critical micelle concentration of given surfactant in aqueous and aqueous salt solutions. **3) X-diffraction analysis** To determine crystal structure of cubic system by X-ray diffraction technique. **4) Polarography** To determine half wave potential of a given ion using half height method, differential method and wave equation method. **Case study** **Any other suitable experiments may be added.**	

Course Outcome: Student should be able to

1) explain and handle the abovementioned instruments
2) calculate various thermodynamic parameters relevant to electrochemical reactions.
3) determine the crystal structures of simple cubic system.
4) calculate and illustrate chemical kinetics, thermochemistry and various physical properties.

MPCP-306 Physical Chemistry Practical Course-V (Lab-V)

Course Objectives: Student will be able to

1) understand the instrumental analysis.
2) learn about determining thermodynamic parameters for electrochemical reactions.
3) study the latent heat of fusion of any compounds.
4) understand the concepts of equivalence conductance of electrolytes, pK values, and molecular weight

Credits = 4	**SEMESTER-III** **MPCP-306 Physical Chemistry Practical Course-VI (Lab-VI)**	**No. of hours per unit/ Credits (60)**
I	**Potentiometry, Spectrophotometry and Conductometry**	
	I) Potentiometry Determination of Thermodynamic Parameters for electrochemical reactions. (To determine G^o, H^o and S^o for the formation of 1 mole cadmium in 1 wt. % amalgam at 25^o C and activity coefficient of solution). **II) Spectrophotometry** 1) To determine stoichiometry & stability constant of ferric Sulphosalicylic acid/ salicylic acid complex by Job's Method and mole ratio method spectrophotometrically. 2) To determine equilibrium constant of reaction $KI + I_2 \rightleftharpoons KI_3$ spectrophotometrically **III) Conductometry** To determine equivalent conductance at infinite dilution of strong electrolytes and weak acid by using Kohlrausch Law and dissociation constant for weak acid conductometrically.	
II	**Cryoscopy, latent heat of fussion, thermochemistry and pH metry**	
	IV) Cryoscopy To determine molecular weight and state of benzoic acid in benzene. **V) Latent heat of Fusion** Determination of latent heat of fusion of a given solid. **VI) Thermochemistry** Determination of heats of dilution and integral heat of solutions. **VII) pH - Metry** To determine dissociation constant of carbonic acid pH metrically.	

	Research project work	

Any other suitable experiments may be added.

Course Outcome: Student should be able to

1) explain and handle the abovementioned instruments.
2) calculate different thermodynamic parameters useful in electrochemical reactions.
3) calculate and illustrate thermochemistry and various physical properties.
4) determine equivalence conductance of electrolytes, pK values of indicators and molecular weight of compounds.

References: -

1) C. N. Banwell, Fundamentals of molecular spectroscopy, MCGRaw-Hill Book company 4th edition, 1972. [Unit I]
2) A. M. James and F. E. Prichard, Practical of physical chemistry, 3rd edition 1974. [Unit I, II]
3) F. Daniels and J. Williams, Experimental Physical Chemistry, 2nd edition, 1935. [Unit I, II]
4) R. C. Das and B. Behera, Experimental Physical Chemistry, Tata McGraw-Hill, 1983. [Unit I, II]
5) B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, 2015. [Unit I, II]

M. Sc. II Semester IV

MPCT-401: Thermodynamics and Molecular Modelling

Course Objectives: Student will be able to

1. study the modern and classical quantum principles.
2. understand the statistical and molecular mechanics.
3. learn the different molecular dynamic simulation methods.
4. understand the role of non-equilibrium in thermodynamics.

Credits = 4	**SEMESTER-IV** **MPCT-401: Thermodynamics and Molecular Modelling**	**No. of hours per unit/ credits**
UNIT I	**Modern Theoretical Principles**	**(15)**
	Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and minima. Integrating factors,	

	Paff differential equations, Caratheodary's theory. Legendre transformations. Derivation of thermodynamic identities. The second law of thermodynamics, classical formulations, mathematical consequences of second law. Entropy changes, Clausius inequality. Free energy concept. General condition of equilibrium. Thermodynamic potentials.	
UNIT II	**Statistical and Molecular Mechanics**	**(15)**
	Ensembles, ensemble average and time average of the property, ergodic hypothesis, partition functions and thermodynamic properties, classical and quantum statistics, properties of photon gas, thermodynamic properties bosons, use of quantum statistics for evaluation of absolute entropies, condensation of helium, Fermi energy, electron gas in metals. Heat capacity of solids, Einstein and Debye specific heat equations. Characteristic temperatures. Debye T^3 law **(08)** **Molecular Mechanics:** Introduction, the Morse potential model, harmonic oscillator model, force fields development, various energy terms and non-covalent interactions included in force fields, Lennard-Jones type and truncated Lennard-Jones potentials, Kihara potential, commonly used force fields, parameterization, introduction to software packages used for performing molecular mechanics. **(07)**	
UNIT III	**Molecular Dynamic Simulation Methods**	**(15)**
	Introduction, microscopic and macroscopic properties, time scale of chemical/biological process, force field methods, bonded and non-bonded interactions, advantages and limitations of Force Field Methods, molecular dynamics methods, neighbour searching, Trotter decomposition, cut-offs, temperature and pressure coupling methods, integration algorithms: Verlet algorithm, Leap-frog algorithm, Velocity Verlet, Beeman's algorithm, Constraint algorithms: shake, lincs, etc., Stochastic and Brownian dynamics, topology files, energy minimization: steepest descent method, conjugate gradient method, L-BFGS. Solvent models, Solvation, implicit and explicit solvation, heating dynamics, equilibration dynamics, production dynamics, trajectory analysis, particle mesh Edward dynamics, boundary conditions, Exclusions and 1-4 interactions, gradient based methods, steepest descent method, conjugate gradient method, replica exchange method, conformational analysis, normal mode analysis, free energy calculation: free energy perturbation method, thermodynamic	

	integration method, thermodynamic cycles for free energy calculations, determination of hydration/solvation free energy, protein folding free energy, protein-ligand binding free energy etc. Software packages for performing Monte-Carlo and Molecular dynamic simulation as well as for visualization and analysis trajectories	
UNIT IV	**Non-equilibrium thermodynamics**	**(15)**
	Conversion of mass in closed and open systems, conservation of energy in closed and open systems. Law of increasing entropy. Non-adiabatic process and clausius inequality, steady state. Thermodynamic equations of motion. Chemical and electrochemical affinities. Coupling reactions. Rates and affinities. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients. Concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Entropy production in closed and open systems. Entropy production due to heat flow. Chemical potentials. Diffusion, electromotive force, electro-osmosis, thermoelectric effect and other reactions involving cross relations. Onsagar reciprocity theory, Gibbs equations, postulates and methodologies.	

Course Outcomes: Student should be able to

1) clarify the modern and classical quantum principles.
2) explain basics concepts of statistical and molecular mechanics.
3) compare the different molecular dynamic simulation methods.
4) explain the role of non-equilibrium in thermodynamics.

References: -

1) Ira N. Levine, Quantum Chemistry, (Pearson, City University of New York), 6th edition, 2019. [Unit I]
2) Gurdeep Raj, Advanced Physical Chemistry, (Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)) 3rd edition, 2020. [Unit II, III, IV]
3) S. N. Blinder, Advanced physical Chemistry, The Macmilan Company, 1967. [Unit I, II]
4) L. K. Nash, Elements of statistical thermodynamics, 2nd Edition, Addison Wesley, 1974. [Unit II]

(Additional reading)

5) Online Manuals for simulation and visualization packages such as GROMACS, VMD,NAMD, AMBER, TINKER, etc. [Unit III]
6) R.P. Rastogi, Introduction to Non-equilibrium Physical Chemistry: Towards Complexity andNon-linear Science, Elsevier, Oxford, 2008. [Unit II]

MPCT-402 Chemical Kinetics

Course Objectives: Student will be able to

1) study the kinetics of fast reactions and their techniques.
2) comparative study of various theories of reaction rate.
3) understand the value of heterogeneous catalysis for feasibility of reaction.
4) study the Hammett plots and Hammett equation in details.

Credits = 4	**SEMESTER-IV** **MCT-P-402 Chemical Kinetics**	**No. of hours per unit/ credits**
UNIT I	**Fast Reactions**	**(15)**
	Kinetics of Fast reactions: Relaxation techniques, pressure jump and temperature jump methods, NMR relaxation, flash photolysis and molecular beam methods. Hydrogen ion dependence of reaction rates: Protonation and hydrolysis equilibria, determination of active reactant species forms kinetic data, interpretation of hydrogen ion effect with example.	
UNIT II	**Theories of Reaction Rate**	**(15)**
	Equilibrium and rate of reaction, Partition function and activated complex, Collision theory of gas reaction, collision frequency. The rate constant , molecular diameters , collision theory vs. experiment Transition state theory (Thermodynamic and partition function approach) Activated complex theory of reaction rates, reaction coordinate and transition state, formation and decay of activated complex, Eyring equation, thermodynamic aspects, Theory of unimolecular reactions.	
UNIT III	**Heterogeneous Catalysis**	**(15)**
	Reactions at solid surfaces-Adsorption and desorption, competitive adsorption, catalysis, unimolecular and bimolecular surface reaction. ACT of surface reactions, surface diffusion, temp programmed desorption and modulated molecular beam method. Heterogeneously catalysed oxidation and reduction reactions: oxidation of hydrogen with oxygen (Determination of Pt, Pd, Ir and Rh) Reduction of silver bromide (Determination of S and Se), Trace metal ion catalysis and their mechanisms. Micellar catalysis, Berezini, Menger-Portonoy, cooperative and pseudo-phase ion exchange models and examples.	

UNIT IV	**Organic Reaction Mechanisms**	**(15)**
	Linear free energy relationships: Hammett plots, Hammett equation, substituent and reaction constants and their physical significance, calculation of k and K values, Yukawa- Tsuno equation. Taft equation, steric parameters Solvent effects, Grunwald-Winstein equation.	

Course Outcomes: Student should be able to

1. calculate rates of reactions by using various kinetic techniques.
2. compare studies on various theories of reaction rates.
3. understand the role of heterogeneous catalysis in feasibility of reaction.
4. calculate various parameters such as substituent and reaction constants.

References: -

1) K. J. Laidler, Chemical Kinetics, 3rd edition, 1965. [Unit I, III, IV]
2) A. A. Frost and R. G. Pearson, Kinetics and Mechanismby, 2007. [Unit I, II]
3) B. S. Bahl, G. D. Tuli, Essential of physical chemistry, revised edition 2008. [Unit II]
4) K. J. Laidler, Theory of chemical reaction rates, McGrew Hill, New York, 1969.
5) J. N. Bradley, Fast Reactions, Clarendon Press Oxford, 1974. [Unit I]
6) Asim K. Das, Micellar effect on the kinetics and mechanism of chromium (VI) oxidation of organic substrates, Coordination Chemistry Reviews, Vol. 248, p 81-89, 2004. [Unit III]

MPCT-403-Molecular structure-II

Course Objectives: Student will be able to

1) study the various electrical properties of molecules.
2) comprehend the magnetic properties of molecules.
3) learn the fundamentals of nuclear magnetic resonance spectroscopy.
4) study the mossbauer spectroscopy and electron spin resonance spectroscopy.

Credits = 4	**SEMESTER-IV** **Molecular structure-II**	**No. of hours per unit/ credits**
UNIT I	**The Electric Properties of Molecules**	**(15)**
	Electric dipole moment of molecule, polarization of a dielectric, polarizability of molecules, Clausius-Mossotti equation. Debye equation, limitation of the Debye theory, Dipole moment and ionic	

	character, Bond moment, Group moment, vector addition of moments, bond angles, the energies due to dipole-dipole, dipole induced dipole and induced dipole-induced dipole interaction. Lennard-Jones potential. Dielectric breakdown, piezoelectricity, ferroelectrics.	
UNIT II	**The Magnetic properties of Molecules**	**(15)**
	Diamagnetism and Para magnetism. Volume and mass susceptibilities. Lengevins classical theory of diamagnetism and paramangnetism Atomic and ionic susceptibility. Pascal constants, Curie - Weiss law. Van Vleck general equation of magnetic susceptibility. Determination of magnetic susceptibility. Ferro and ferri magnetism, application to coordination complexes and complex ions of transition metals.	
UNIT III	**Nuclear Magnetic Resonance Spectroscopy**	**(15)**
	The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels, The larmor precession. relaxation times. the meaning of resonance and the resonance condition. NMR experiment, singnificance of shielding constants and chemical shift. The origin and effect spin - spin coupling, factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena, ^{13}C NMR spectroscopy, double resonance and nuclear-overhauser effect.	
UNIT IV	**Electron Spin Resonance Spectroscopy & Mossbauer Spectroscopy**	**(15)**
	A) Electron Spin Resonance Spectroscopy Electron spin and Magnetic moment, Interaction of electron spin with external magnetic field, Resonance condition in ESR and significance of 'g' value. ESR spectra of organic free radicals, McConnell relation, Jahn-Teller theorem, Electron Exchange reactions, applications of ESR. **B) Mossbauer Spectroscopy** Basic principle of Mossbauer spectroscopy, hyperfine structure, quadrupole splitting, instrumentation and applications of Mossbauer spectroscopy, Problems related to Mossbauer spectra.	

Course Outcomes: Student should be able to

1) calculate various parameters of electric properties of molecules

2) determine the magnetic properties of a variety of molecules.
3) describe the basic concepts of nuclear magnetic resonance spectroscopy.
4) explore Mossbauer and ESR Spectroscopy applications.

References: -

1) C. N. Banwell, Fundamentals of molecular spectroscopy, MCGRaw-Hill Book company 4th edition, 1972. [Unit I, III, IV]
2) P. W. Atkin, Physical Chemistry, ELBS, 4th edition, 1986. [Unit I, II, III, IV]
3) G. M. Barrow, Introduction to molecular spectroscopy, Gordon M. Publication, 1962. [Unit I, II, III, IV]
4) J. D. Roberts, Nuclear magnetic Resonance, McGrawHill, 1967. [Unit III]
5) M. Davies, Electrical and optical properties of molecular behavior, pergman press.1 st edition 1965. [Unit I]

Elective Papers:

MPCT--404 A :Physicochemical Techniques

Course Objectives: Student will be able to

1) learn about various X-ray techniques as well as their applications.
2) study about the fundamentals of XPS and mass spectroscopy.
3) understand the neutron activation analysis in details.
4) comparative study of several physicochemical techniques such as TGA, DTA and DSC.

Credits = 4	**SEMESTER-IV** **MCT-P-404 A: Physicochemical Techniques**	**No. of hours per unit/ credits**
UNIT I	**X-ray methods**	**(15)**
	Generation and properties of X-rays, generation of X-rays, -spectra, X-ray absorption, Concept of absorption edge, application, X-ray absorptive apparatus, radiography and radiotherapy, applications, X rays fluorescence, fundamental principles, instrumentation, wavelength dispersive and energy dispersive, quantitative analysis, X-ray emission, fundamental principles, X ray diffraction, powder diffractometer, applications in material science, electron microprobe, further advanced techniques.	

UNIT II	**XPS (X-ray photoelectron spectroscopy) and Mass spectrometry)**	**(15)**
	Theory satellite peaks, chemical shift, apparatus, chemical analysis, using ESCA, AES- fundamental principles UP Luminescence, chemiluminescence, gas phase, liquid phase chemiluminescence, apparatus, bioluminescence, electrochemiluminescence **Mass spectrometry:** Theory, instrumentation-basic components, ionization sources, analyzers, resolution, chemical analysis, advanced techniques-GC/MS, MS/MS introduction	
UNIT III	**Neutron Activation Analysis**	**(15)**
	Principle, target, matrix, cross-section, fluxes, saturation activity, excitation function, Different steps involved in NAA, radiochemical and instrumental NAA, prompt radiation and pulse neutron activation analysis, applications	
UNIT IV	**A) Inductively coupled plasma atomic emission spectroscopy(5L)** Principle, instrumentation, analysis and applications **B) Thermal methods of analysis: (6L)** TGA, DTA, DSC and thermometric titrations – principle, instrumentation, factors affecting TGA curve, applications **C) Radiometric titrations: (4L)** Principle, types and instrumentation	**(15)**

Course Outcomes: Student should be able to

1. describe several types of X-ray techniques.
2. explain in detail the fundamentals of XPS and mass spectroscopy.
3. describe how neutron activation analysis can be used in science.
4. compare and contrast TGA, DTA, and DSC methods.

References: -

1) R. D. Braun, Introduction to Instrumental Analysis, Pharmamed Press, Indian Reprint, 2006. [Unit I, II, III, IV]
2) D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5th edition, Philadelphia Saunders College Publishing,1988. [Unit I, II, III, IV]
3) P. Kruger, Principles of activation analysis, John Wiley, 1971. [Unit III]
4) J. Tolgyessy and S. Verga Nuclear analytical chemistry- Vol. 2, University Park press, 1972. [Unit III, IV]

MPCT-404-B : Surface Chemistry

Course Objectives: Student will be able to

1) understand the surface chemistry of interfaces.
2) learn B. E. T. equation and methods of determination of surface area.
3) understand the fundamentals of colloids and emulsion in great depth.
4) study the solid-liquid and solid - solid interfaces.

Credits = 4	**SEMESTER-IV** **MCT-P-404 B: Surface Chemistry**	**No. of hours per unit/ credits**
UNIT I	**Surface Chemistry of interfaces**	**(15)**
	Types of interfaces, Liquid-vapour interface, Surface tension and interfacial tension, surface tension across curved surfaces, capillary action, methods of determination of surface tension, vapor pressure of droplet (Kelvin equation), Surface activity and adsorption phenomenon, Trube's Rule, Gibb's Adsorption equation, liquid-liquid interfaces, work of cohesion and adhesion, surface spreading , spreading of one liquid on the surface of other liquid, spreading coefficient and derivation for its relation with surface tension, monomolecular films, preparation of monolayer films, Langmuir-Boldget method, physical states of films, ideal equation of states, experimental aspects based on use of Langmuir-Adam surface pressure balance,	
UNIT II	**Solid-gas interfaces**	**(15)**
	Adsorption of gases on solids, factors affecting adsorption, Experimental methods of determining gas adsorption, volumetric method, Gravimetric method, types of adsorption isotherms, The B.E.T. equation, methods of determination of surface area, Herkins's Jura method, BET method, Point B Method, Heat of adsorption, Calorimetric method of determination of heat of adsorption, Chemisorption, Kinetics of chemisorptions, Heterogeneous catalysis (Contact catalysis), mechanism of catalysis, factors influencing catalytic activity.	
UNIT III	**Colloids and emulsion**	**(15)**
	The Colloidal state: Introduction, types, preparation and stability of colloids, properties of colloids. Emulsion: Types of emulsion, theories	

	of emulsion and emulsion stability, identification of emulsion types, inversion emulsion, microemulsion: theory and application, micellisation, structure of micelle, reverse micelle, solubisation of water insoluble organic substances.	
UNIT IV	**Solid-Liquid and Solid - Solid interfaces**	**(15)**
	Solid-liquid interfaces, Introduction, wetting phenomenon, contact angle and wetting, heat of wetting, methods of determination of contact angle, contact angle hysteresis, wetting agents, selective wetting, applications in detergency, and pesticide affectivity, Solid-Solid interfaces, introduction, Surface energy of solids, adhesion and adsorption, sintering and sintering, mechanism, Tammann temperature, importance of impurities, surface structure and surface composition. Friction and lubrication, mechanism of lubrication, solid state lubricants.	

Course Outcomes: Student should be able to

1) calculate different parameters of surface chemistry.
2) derive B. E. T. equation.
3) decide the specific applications of emulsion and colloids.
4) compare the solid-liquid and solid - solid interfaces.

References: -

1) S. J. Gregg, The Surface Chemistry of Solids, Chapman & Hall Ltd. London, Second Edition, 1961. [Unit I, II, III, IV]
2) Gurdeep Raj, Advanced Physical Chemistry, Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP), 2009. [Unit I]
3) B. R. Puri, L. R. Sharma & M. S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co., Jalander-144008, 2020. [Unit I, II, III, IV]
4) S. Pahari, Physical Chemistry, New Central Book Agency (P) Ltd. Kolkata, 2nd edition, 2007. [Unit I, II, III, IV]
5) S. J. Gregg and K. S. W. Sing, Adsorption, surface area and porosity, Academic press ltd. London, 1967. [Unit I, II, IV]

MPCP--405 PRACTICAL COURSE – IV: LAB VII

Course Objectives: Student will be able to

1) study the characterization of complexes by different techniques.
2) study the indicator constant and isobestic point of dyes.
3) learn the different methods of synthesis of nanoparticles.

4) study the application of metal and metal oxides nanoparticles for environmental remediation.

Credits = 4	**SEMESTER-IV** **MCP-P-405 PRACTICAL COURSE – IV: LAB VII**	**No. of hours per unit/ Credits (60)**
I	**Spectroscopy study**	
	1) Characterization of the complexes by electronic and IR spectral data. 2) Determination of indicator constant and isobestic point of an indicator. 3) Determination of stability constant of ferric thiocyanate complex.	
II	**Synthesis of Nanomaterial's**	
	1) To synthesize metal nanoparticles and to study their size-dependent optical properties 2) 'Green' synthesis of metals and their oxide nanoparticles: applications for environmental remediation 3) To synthesize carbon nanoparticles. 4) To synthesize carbon nanoparticles and study adsorption behavior of dye. **Case study**	

Any other suitable experiments may be added

Course Outcome: Student should be able to

1) characterize complex molecules by spectroscopically.
2) calculate indicator constant and isobestic point of various dyes.
3) synthesize nanoparticles with different size.
4) prepare metal and metal oxides nanoparticles for applications of environmental remediation.

MPCP--406 PRACTICAL COURSE – IV: LAB VIII

Course Objectives: Student will be able to

1. understand rate of chemical reaction by different approach.
2. learn the HPLC instrument for analysis of samples.
3. comparative study of synthesis of thin film by different techniques
4. study the characterization of thin film.

Credits=4	SEMESTER-IV MCP-P-406 PRACTICAL COURSE – IV: LAB VIII	No. of hours per unit/ Credits (60)
I	**Kinetic study and Industry oriented Practical's**	
	1. Spectrophotometric method 2. Conductometric method. 3. Industry oriented Practical's	
II	**Preparation of Thin film and HPLC analysis**	
	1. Preparation and characterization of thin film 2. To synthesize thin film and study their optoelectronic properties 3. Analytical study of medicinal plants via HPLC **Research project work** **Study tour**	

Any other suitable experiments may be added

Course Outcomes: Student should be able to

1) calculate rate of reaction by different techniques.
2) explain the operating system of HPLC instrument.
3) synthesize thin film by different methods.
4) characterize thin film.

References: -

1) C. N. Banwell, Fundamentals of molecular spectroscopy, MCGRaw-Hill Book company 4th edition, 1972. [Unit I]

2) A. M. James and F. E. Prichard, Practical of physical chemistry, 3rd edition 1974. [Unit I, II]

3) F. Daniels and J. Williams, Experimental Physical Chemistry, 2nd edition, 1935. [Unit I, II]

4) R. C. Das and B. Behera, Experimental Physical Chemistry, Tata McGraw-Hill, 1983. [Unit I, II]

5) B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, 2015. [Unit I, II]