M.Sc. Semester I

	The Maharaja Sayajirao University of Baroda Faculty of Science Department of Chemistry Sayajigunj , Vadodara 390002, 0265-2791891,	ACADEMIC YEAR 2018-2019

Bachelor of Science (Hons.) Chemistry

YEAR	I	**CORE**	Credit	3
Semester	I	**Course CHE2101** **Inorganic Chemistry-1**	Hours	45

OBJECTIVES:

COURSE CONTENT / SYLLABUS

UNIT-I	*Fundamentals of Quantum mechanics:* Postulates of quantum mechanics, interpretation of wave function, properties of wave function, hermitian operators, expectation energy and mean value theorem. Particle in a box, quantum mechanical tunneling, quantum well, degeneracy of energy levels H-atom wave function, separation of translational and rotational parts of the Schrödinger equation, separation of radial and angular equations, solution of R(r), Θ(θ), Φ(φ) equations. Quantum numbers and their significance, shapes of the orbitals, energy of H-atom orbitals.
UNIT-II	*Quantum mechanics and multielectronic atoms:* Multielectronic atoms, wave functions, Self-Consistent Field, Hartree-Fock method. Energy levels in multielectronic atoms and ground spectral states. Spectral states of olyelectronic atoms, LS and jj couplings, allowed microstates of d electrons and spectral states. Racah and Slater parameters and their relationship with energies of spectral states, Zeeman and Stark effects. Spectra of alkaline earth metal ions. Electrostatic concept of complex formation, effect of ligand field geometry on the energy of d-orbitals, factors affecting crystal field splitting, spectrochemical series, Jahn -Teller Theorem.
UNIT-III	*Metal-Ligand equilibria:* Metal-ligand equilibria in solution, stepwise and overall formation constants and their interpretation, trends in stepwise formation constants. Factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and macrocyclic effect. Determination of stoichiometry of complex formation, Determination of binary formation constants of complexes by pH - metry and spectrophotometry. Stability of mixed ligand complexes, astatistical stabilization, ring-size effect, inter ligand electron delocalization, intramolecular inter ligand interactions and their effect on the stability of ternary complexes.

REFERENCES

1. Theoretical Inorganic Chemistry, M. C. Day and J. Selbin, Van Nostrand-Reinhold
2. Electron and Chemical bonding, H.B. Gray Benjamin, New York
3. Atomic Structure and Chemical Bonding , Manas Chanda McGraw Hill, New Delhi
4. Introduction to Atomic and Molecular Structure, J. Bartlet, John-Wiley & Sons, New York
5. The Chemical Bond , J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley, London
6. Advanced Inorganic Chemistry , F. A. Cotton and G. Wilkinson, Wiley, London
7. Coordination Chemistry, Martell and Kelvin , Academic Press.
8. Coordination Chemistry, D. Banerjea, Tata McGraw Hill
9. Advanced Inorganic Chemistry, Series Vol.1-10, A.G.Sharp, Academic press
10. Inorganic Chemistry, J. E. Huhey, Harper International SI Edition.

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Bachelor of Science (Hons.) Chemistry				
YEAR	I	**CORE**	Credit	3
Semester	I	**Course CHE2102** **Organic Chemistry-1**	Hours	45
OBJECTIVES:				

COURSE CONTENT / SYLLABUS

UNIT-I	*Aliphatic nucleophilic substitution reactions:* :The $S_{N}1$, $S_{N}2$, and $S_{N}i$ reactions, their mechanisms and stereochemistry, leaving group effect and reaction medium, ambiedent nucleophile, Neighboring group participation (anchimeric assistance), Aliphatic electrophilic substitution reactions $S_{E}1$, $S_{E}2$ and $S_{E}i$ reactions, their mechanism and stereochemistry. Aliphatic addition reactions, electrophilic and nucleophilic addition reactions, mechanism, stereochemistry of additions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity, addition to cyclopropane ring.
UNIT-II	*Organic reaction mechanisms*: Mechanism, Types of reactions, thermodynamic and kinetic requirements, Potential energy diagram. Energy of activation, Transition state & intermediate, methods of determining mechanism, primary and secondary isotope effects, solvent effects, substituent effects. Effect of structure on reactivity, Hammett equation, linear free energy relationship. Substituent constant, reaction constant, correlation of change in reaction constant with mechanism, Taft equation.
UNIT-III	*Molecular rearrangements*: Mechanism to nucleophilic, electrophilic, and free radical molecular rearrangements. Carbon-carbon rearrangements: Wagner-Meerwein, Tiffeneau-Demyanov, Favorskii, Wolff, Benzil-Benzilic acid, Neber, Benzidine rearrangements, Carbon-nitrogen rearrangements: Hoffmann, Curtius, Lossen Schmidt and Beckmann rearrangements. Carbon-oxygen rearrangements: Bayer-Villiger, Dakin and Wittig rearrangements.

REFERENCES

1. Advanced Organic Chemistry , Jerry March
2. Physical Organic Chemistry, Jack Hine
3. Organic Chemistry, Stanley H. Pine
4. The Modern Structural Theory of Organic Chemistry , L.N. Ferguson
5. Comprehensive Organic Chemistry -D. H. R. Barton Vols.1-6
6. Organic Chemistry -R.T. Morrison and R. N. Boyd, 6th Edition
7. Guidebook to Mechanisms in Organic Chemistry, P. Sykes
8. Synthetic Approaches in Organic Chemistry, R. K. Bansal
9. Reaction Mechanisms in Organic Chemistry, S. M. Mukherjee and S. P. Singh
10. Understanding Organic Reaction Mechanisms , Adam Jacobs
11. Organic Reaction Mechanisms, V.K. Ahluwelia, R.K. Parashar, Narosa. 2002
12. Vogel's Textbook of Practical Organic Chemistry, Revised by B. S. Furniss, A.J. Hannaford, P.W.G. Smith, A. R. Tatchel.

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Bachelor of Science (Hons.) Chemistry				
YEAR	I	**CORE**	Credit	3
Semester	I	**Course CHE2103** **Physical Chemistry-1**	Hours	45
OBJECTIVES:				

COURSE CONTENT / SYLLABUS

UNIT-I	*Kinetic Theory of Gases:* Derivation of Maxwell's distribution law for molecular velocity and its applications in calculating molecular speeds: Most probable, average and root mean square. Intermolecular collisions, frequency of collision, Molecular collision and mean free path. Collision theory of reaction rates. Transport process: Thermal conductivity, kinetic theory of thermal conductivity of gases, viscosity, flow rate of fluids, measurement of viscosity of gases, relation between viscosity and mean free path of gases, effect of temperature on viscosity of gas. Diffusion of gases.
UNIT-II	*Chemical Kinetics:* Recapitulation. Complex Reactions: Reactions approaching equilibrium, steady state approximation, Rate laws for consecutive, opposing and parallel reactions, explosive reactions. Techniques to study gas phase reactions. Fast reactions; relaxation, stop flow and flash photolysis. Kinetics of enzyme reactions. Harpoon mechanism (Molecular Beam method). Activated complex theory: Reaction coordinate and the transition state, potential energy surface, concentration of activated complex and rate constant, experimental observation of activated complex. Thermodynamic aspect. Theories of unimolecular reactions: Lindemann and Hinshelwood. Third order reaction
UNIT-III	*Surfactants and solution behavior:* Introduction of liquid surfaces and source of surface tension/interfacial tension. Methods of surface tension measurement Classification of surfactants, micellization, factors influencing CMC. Thermodynamics of micellization. Aggregation number and its determination, micellar solubilization, micro emulsion, reverse micelles, applications of various surfactant organized assemblies

REFERENCES

1. Laidler,K. J., (1987)*Chemical Kinetics*, Third Edition, Pearson Education, Noida (India)
2.Levine, R.D., *Molecular reaction Dynamics*, (2009), Cambridge University Press, NY. (Paperback Edition)
3. Raja Ram J. and Kuriacose J.C., (1993).*Kinetics and Mechanism of Chemical Transformations,* MacMillan Indian Ltd., New Delhi
4.Rakshit, P. C., (2004)*Physical Chemistry*, Seventh Edition, Sarat Book Distributors, Kolkata
5. Moroi, V., *Micelles: Theoretical and Applied Aspects*, Plenum Publishers, New York.
6. Rosen, M.J. (1989) *Surfactants and Interfacial Phenomena*, Wiley, NewYork.
7. Levine,I.N., (2002) *Physical Chemistry*, Fifth Edition, Tata McGraw Hill Pub.Co. Ltd., New Delhi.
8. Engel, T. and Reid, P., (2007) *Physical Chemistry*, First Edition, Pearson Education, Noida
9. Ball, D. W., (2003) *Physical Chemistry*, India Edition Thomson Learning, USA
10. Atkins P. and De Paula J., (2006)*Atkins' Physical Chemistry*, Eighth Edition, Oxford University Press, New York.

M.Sc. Semester I

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Bachelor of Science (Hons.) Chemistry			
YEAR	I	**CORE**	Credit 3
Semester	I	**Course CHE2104** **Advanced Analytical Chemistry-I**	Hours 45
OBJECTIVES:			

COURSE CONTENT / SYLLABUS

UNIT-I	**Basics of Electroanalytical and Chromatographic Techniques** *a) Electrochemical methods:* Definitions and terminology involved in electrochemistry. *Specific ion selective electrodes:* Glass electrode for H^+ / Na^+ ions, solid membrane electrode for fluoride, liquid membrane electrode for calcium. Enzyme - substrate electrode for NH_3, and gas sensing electrodes for SO_2/ NH_3/CO_2 / O_2. Introduction to Amperometry and Non - aqueous titrations. *b) Chromatography:* Column theory (qualitative approach), mechanism of separation and applications of adsorption, partition, ion exchange, affinity and size exclusion chromatography. Qualitative and quantitative analysis by chromatography
UNIT-II	*GC and HPLC* *Introduction to Gas Chromatography: Instrumentation, types of columns, injection systems and detectors. Capillary GC, GCMS. Introduction to super critical fluid chromatography (SFC). Liquid Chromatography: Principles, solvent delivery systems, injections system, detectors and columns. Size-exclusion chromatography.*
UNIT-III	*Thermal methods:* *Thermogravimetry analysis: Principle, construction and working of thermobalance, factors affecting TGA, Applications of TGA.Differential thermal analysis and differential scanning calorimetry: Principle, Instrumentation, factors affecting analysis and applications. Thermo mechanical analysis [TMA] Instrumentation and application, thermometric titrations.*

REFERENCES

1. An Introduction to separation science, L.R. Snyder and C. Horvath, Wiley Interscience
2. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman 5th edition (1998), Saunders College Publishing, Harcourt Brace & Company, U.S.A
3. Electrochemical Methods: Fundamentals and Applications, A.J. Bard and L.R. Faulkner 2nd Edition (2000), Wiley, New York.
4. Fundamentals of Electroanalytical Chemistry, P Monk, John Wiley, NY.
5. Instrumental Analysis , Y.H. Bauer, G.D. Christian, S.E. O'reilly, Allyn and Bacon Inc.
6. Introduction to Thermogravimetric Analysis, C.J. Keattch and D. Dollimore.
7. Working with Ion selective Electrodes, O.K. Camman.

M.Sc. Semester I

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Bachelor of Science (Hons.) Chemistry				
YEAR	I	**CORE**	Credit	3
Semester	I	**Course CHE2105** **Spectroscopy-I**	Hours	45
OBJECTIVES:				

COURSE CONTENT / SYLLABUS

UNIT-I	*Symmetry and Group theory:* Symmetry elements and operations, representation of symmetry operations as matrices, definition of groups, sets of symmetry operations of molecules satisfying the conditions of a group, generators. Axial, non-axial and special point groups.
UNIT-II	Classes of operations, reducible and irreducible representations. Great orthogonality theorem, Derivation of character tables of C_{2v} and C_{3v} point groups. Projection operators and direct products. Transformation properties of atomic orbitals.
UNIT-III	*NMR Spectroscopy:* Nuclear spin, nuclear resonance, saturation, relaxation, Basic instrumentation shielding and deshielding of magnetic nuclei, coupling constant, chemical shift and its measurements. Factors affecting chemical shift, spin - spin interactions and spin decoupling, Introduction to ^{13}C - NMR and FTNMR *Electron Spin Resonance:* Introduction, Instrumentation, electronic spin states in 1 and 2 electron systems, fine structure, applications
UNIT-IV	*X-ray Diffraction:* Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structure al analysis of crystals, index reflections, identification of units cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density. *Electron diffraction:* Theory, measurement techniques and elucidation of structure of simple molecule s. Low energy electron diffraction. *Neutron diffraction:* Scattering of neutrons by solids & liquids. Measurement techniques, Elucidation of magnetically ordered unit cell.

REFERENCES

1. Physical Methods in Chemistry : R.S. Drago, Saunders College
2. Chemical applications of Group Theory , F. A. Cotton Wiley-Eastern, New Delhi
3. Symmetry in Chemistry, H. H. Jaffe and M. Orchin Wiley, New York
4. Group Theory and its Chemical Applications , P.K. Bhattacharya, Himalaya, New Delhi
5. Molecular Symmetry and Group Theory, R.L. Carte, Wiley
6. X- Ray methods : Clive Whiston, John Wiley & Sons.
7. Solid State Chemistry and its Applications, A.R.West, John Wiley & Sons, New York (1984)
8. Instrumental Analysis, D. A. Skoog, F.J.Holler and S.R. Crouch, Thomson Brooks/Cole, Cengage Learning, UK
9. Molecular Structure and Spectroscopy - G. Aruldhas, Prentice Hall of India