	The Maharaja Sayajirao University of Baroda Faculty of Science, Department of Mathematics, Sayajigunj , Vadodara 390002, 0265-2795329, Ext:336, hrkrmaths@gmail.com	ACADEMIC YEAR 2018-2019

Master of Science : Regular

YEAR	I	**CORE:**	CREDIT	3
Semester	II	**CHE2201: Inorganic Chemistry-II**	HOURS	**45**

OBJECTIVES:	The objective of this course is to equip the students with detailed understanding of various types of interactions between molecules in simple compounds to clusters and inorganic polymers. The covalent bonding in molecule is discussed in detail. M-M bond formation, metal clusters and bonding in inorganic ring compounds and polymers is discussed in detail. This is expected to develop a clear understanding of structure property relationship which can further enable the students in understanding and predicting spectroscopic properties and chemical reactivity of various molecules.

COURSE CONTENT / SYLLABUS

UNIT-I	**Chemical Bonding:** Variation and linear combination principles, valence bond and molecular orbital interpretations of H_{2+} and H_2 molecules. Valence bond and molecular orbital interpretation of other diatomic molecules. Stability, bond energy and bond distance, Resonance concept. Directed valency: Pauling - Slater's concept. Valence bond theory: Formation of hybrid orbitals, their wave functions and properties. Symmetry, composition of hybrid orbitals in and formation of linear AB2, triangular AB3, AB4, AB5 and AB6 molecules. Molecular Orbital Theory: Symmetry adapted linear combinations of terminal atom orbitals and formation of molecular orbitals in simple polyatomic compounds with triangular, tetrahedral and square planar geometry.	
UNIT-II	**Molecular geometry:** VSEPR theory. Walsh diagrams. M-M multiple bonds. Structure and bonding in the metal complexes with p -acids, on the basis of spectral evidence. Stabilization of unusual oxidation states. Synthesis, structure and bonding in metal carbonyls and nitrosyls. M-M bonds in metal clusters. Cluster valence electrons and Wade-Mingos-Lauher rules. Structure elucidation based on CVE and spectroscopic data. Isolobal analogies.	
UNIT-III	Multicentric boranes and their topology, carboranes and metallo carboranes. Inorganic Polymers and Ring compounds: Linear and cyclic Borazenes, phosphazenes and thiazenes. Phosphonitrilic polymers. Synthesis, structure and bonding in organoboron,and organo phosphorous.	

REFERENCES

Reference Books:
1. Lee J.D., (1991) Concise Inorganic Chemistry, 4th Edition, Chapman and Hall,
2. Puri B.R., Sharma L.R. and Kalia K.C., (2006). Principles of Inorganic Chemistry, 29th Edition, Milestone Publ., Delhi
3. Cotton F.A. and Wilkinson G., (2009) Basic Principles of Inorganic Chemistry, 3rd Edition, Wiley Eastern,
4. Mahan B.H., (2009) University Chemistry, 3rd Edition, Narosa Publ House, New Delhi.
5. Gilreath E. S., (1985) Fundamental Concepts of Inorganic Chemistry, 2nd Edition, McGraw Hill Int.

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ACADEMIC YEAR 2018-2019

Master of Science : Regular

YEAR	I	**CORE**	CREDIT	3
Semester	II	**CHE2202:** **Organic Chemistry-II**	HOURS	45

OBJECTIVES:	Understanding organic chemistry needs learning the fundamental aspects, which involve aromaticity, reaction mechanism and rearrangements. These topics will be covered in this course.

UNIT-I	Aromaticity: Aromaticity and Huckel's rule, Aromaticity in benzenoid and non-benzenoid compounds, annulenes, fullerenes. Alternant and non-alternant hydrocarbons, energy level of molecular orbitals, antiaromaticity, homoaromaticity,non-aromatic compounds. Concept of Chirality: Recognition of symmetry elements and chiral structures, stereoisomerism, determining absolute configuration. Optical activity and optical purity, Resolution,	
UNIT-II	Reactive intermediates: Structure stability and reactivity of intermediates, Generation and structure of carbocation, the concept of classical and non-classical carbocations, reactions involving carbocations, Carbanion, structure and reactivity, generation and reactions. Structure and reactivity of free radicals, carbenes and nitrenes as intermediates, their structure, generation and reactions. Aryne mechanism and ways of generation and their reactions. Introduction to hetrynes and reactions.	
UNIT-III	Reactions, mechanism and applications of the following name reactions: Reformatsky reaction, Cannizzaro reaction, Claisen reaction,	

	Dieckmann reaction, Dieckmanm-Thorpe reaction, Neber rearrangement, Curtius rearrangement, Schmidt rearrangement.

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	Guidebook to Mechanisms in Organic Chemistry, P. Sykes
6	Reaction Mechanisms in Organic Chemistry, S. M. Mukherjee and S. P. Singh
7	Stereochemistry of Carbon Compounds, E. L. Eliel
8	Stereochemistry of Organic Compounds, D. Nasipuri
9	Name Reactions – A Collection of Detailed reaction Mechanisms, Li Jie Jack, Springer, NY.

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Master of Science : Regular

YEAR	I	**CORE**	CREDIT	3
Semester	II	**CHE2203: Physical Chemistry-II**	HOURS	45

OBJECTIVES:	Study and derivation of isothermal adsorption model for gas-solid system. Synthesis, characterization and application of catalyst.Study of electrical double layer and various model to probe the solid-liquid interphase. Study of corrosion as an electrochemical process and its inhibition. Basic of Statistical thermodynamics and derivation of Boltzmann's distribution law. Application of statistical thermodynamics in evaluating various types of energies of an ideal gases

COURSE CONTENT / SYLLABUS

UNIT-I	Adsorption and catalysis: Heat of adsorption, Langmuir and BET isotherms, estimation of surface area, thermodynamics of chemisorption. General features of homogeneous and heterogeneous catalysis, catalytic activity and strength of chemisorption, promoters and poisons, catalyst support, methods of preparation of heterogeneous catalysts, important industrial catalysts	
UNIT-II	Electrochemistry: Electrical double layer: Structure of electrical interface, parallel plate- condenser model, Gouy-Chapmann diffused charge model, Stern model, limitations of these models. Thermodynamics and kinetics of electrochemical metal deposition and dissolution process (corrosion), mechanism, Local cell theory, corrosion current, Evan's diagram, Protection and prevention of corrosion.	
UNIT-III	Statistical thermodynamics: Limitations of classical thermodynamics. Introduction to the terms like ensemble, population, equipartition of energy, degeneracy. Boltzmann's distribution law, Evaluation of β, partition function, Distinguishable and indistinguishable particles, molar partition function, Electronic, Translational, Rotational and Vibrational partition functions. Sackur-Tetrode equation.	

REFERENCES

1.	Bockris, J. O'M. and Reddy, A. K. N. (1998) Modern Electrochemistry, Vol. 2 A & B, Second Edition, Plenum Press, New York.
2	Chakrabarty, D. K. (Reprint 2007), Adsorption and Catalysis by Solids, New Age International Publishers, New Delhi.
3	Bond, G. C. (1974), Heterogeneous catalysis: Principles and applications Clarendon Press, Oxford
4	Terry L. Hill, (1987)Introduction of Statistical Thermodynamics, First Edition , Dover Publications, New York.
5	M. C. Gupta, (1990) Statistical Thermodynamics, Second edition, New Age International Publications, New Delhi
6	T. Engel and P. Reid, (2007) Thermodynamics: Statistical Thermodynamics and Kinetics, First Edition, Pearson Education, Noida

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ACADEMIC YEAR 2018-2019

Master of Science in Chemistry

YEAR	I	**CORE**	CREDIT	3
Semester	II	**CHE2204:Advanced Analytical techniques-II**	HOURS	45

OBJECTIVES:	**The objectis course is to make the students understand** • what are the sources of error in analytical data, types of error, and corrective measures • Be familiar with various tools in analytical data analysis and computations • Be able to compare statistically sets of analytical experimental data and take decision about reliability of data • Learn about and be able to calculate theoretical straight line for given set of calibration data and errors associated with the calculations • Know the basic principles of coulometry and electrodeposition techniques. • Be aware of the relative advantages and disadvantages of coulometry and electrogravimetry and potential applications of the two techniques • Know the principles of liquid-liquid extraction and understand the effect of pH, separation kinetics and complexation on the extraction process • Understand how laboratory studies within industry, academia, government, or other testing facilities should be planned, performed, monitored, recorded, reported, and archived as set forth by national and international regulatory bodies • Be familiar with the causes of environmental pollution and remediation methodologies • Understand the influence of water chemistry and metal speciation on the toxicity of metals.

COURSE CONTENT / SYLLABUS

UNIT-I	Statistics for chemists Sources of variation in data, confidence limits of mean, Errors in instrumental analysis: Calibration curves, line of regression, errors in slope and intercept.	
UNIT-II	Analytical Techniques	

	Electrogravimetry: Principle, Electrolysis at controlled potentials and electrolytic separations. Controlled potential coulometry, working of coulometer, coulometric titrations and applications.	
UNIT-III	Good Laboratory Practices and Environmental Chemistry GLP Principles, Documentation of laboratory work, Preparation of Standard Operating Procedures (SOPs), Validation of methods, Reporting and documentation of results, Quality Control and Quality Assurance, Types of Quality Standards for laboratories, Total Quality Management, Audits Environmental Chemistry: Chemical Speciation and toxicity of particulate, gaseous and soluble pollutants, remedial measures. Methods of control of industrial air pollution.	

REFERENCES

1.	. Statistics of analytical Chemistry: J. C. Miller & J. N. Miller, 2nd edition, Prentice Hall, Englewood Cliffs, NJ. 1992
2	Statistical Analysis method for chemists - A software based approach. W.P. Gardiner,The Royal Society of Chemistry, 1997.
3	Modern Analytical Chemistry, D. Harvey , McGraw Hill, 2000
4	Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, and Timothy A. Nieman, Seventh Edition, Cengage Learning, 2017.
5	Introduction to Instrumental Analysis, R. D. Brown, McGraw Hill, (1987).
6	Environmental Chemistry A global perspective Fourth Edition Gary W. vanLoon and Stephen J. Duffy, Oxford University Press, (2017).
7	Environmental Chemistry with Green Chemistry, Asim K.Das, Books and Allied (P) Ltd.,2015
8	Environmental Chemistry , A K De, New Age International Publishers, 8th Edition, 2016

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Master of Science : Chemistry

YEAR	I	**CORE** **CHE2205** **Spectroscopy 2**	CREDIT	3
Semester	II		HOURS	60

OBJECTIVES:	The main objective of the course is to make students aware of theoretical aspect of different spectroscopic techniques such as microwave, IR, Raman, electronic, fluorescence and mass spectroscopy. Objective is to understand the principles, instrumentation and applications of rotational,and vibrational spectroscopy, Raman spectroscopy and learn to derive term symbols for diatomic molecules, apply the Franck-Condon principle and explain the effect of solvent on electronic spectra. Understanding the origin of fluorescence and phosphorescence spectra, explain fluorescence quenching, instrumentation and principles of quantitative analysis using IR and UV-Visible spectroscopy will be explored. Objective is to understand the principles, instrumentation and applications of mass spectrometer, the use of ionization techniques based on application, the basic concepts of Fragmentation Rules and its applications. Final objective is to learn structure elucidation of unknown compounds.

COURSE CONTENT / SYLLABUS

UNIT-I	Molecular Spectroscopy: Interaction of electromagnetic radiation with matter and photophysical processes; Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. Microwave spectroscopy: Basic concept, rotation spectra of simple inorganic compounds, Classification of molecules, rigid rotor model, effect of isotopic substitution on transition frequencies & intensities non rigid rotor, Stark effect nuclear and electron spin interaction and effect of external field. Applications of Micro wave Spectroscopy. Infrared Spectroscopy: Linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. Basic Instrumentation, Selection rules, normal modes of vibration, group frequencies, overtones, Fermi resonance, hot bands, factors affecting the band positions and intensities
UNIT-II	Electronic Spectroscopy: Electronic states of diatomic molecules, Molecular term symbols, selection rules for diatomic molecules, Franck- Condon principle and intensities of electronic spectra. Electronic spectra of polyatomic molecules ,

	Absorptions due to ethylenic and carbonyl chromophore, solvent effects on electronic spectra. Fluorescence Spectroscopy: Fluorescence, and phosphorescence, fluorescence quenching: concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photoexcited donor and acceptor systems (FRET). Stern-Volmer relation	
Unit III	Spectrometric Methods of Analysis: Quantitative analysis using IR spectroscopy Quantitative analysis using UV-Visible spectroscopy: Relationship of l max & e max to structure. Instrumentation. Qualitative and Quantitative analysis: Determination of dissociation constant, Keto – enol tautomerism and stoichiometry, Spectrophotometric titrations. Derivative spectrometry, expanded scale spectrometry and reflectance spectrometery. Mass Spectrometric Technique: Introduction to Mass Spectrometry – history and basics ,magnetic sector instruments, Ion cyclotron and time-of-flight instruments, Quadrupoles and tandem MS instruments , Sample inlet systems.	
Unit IV	Mass Ionization techniques: electron impact, chemical ionization, field desorption (FAB),_electrospray , Interpretation of spectra. Structural elucidation of simple molecules using spectral data: Molecular Formulae Index (D.B.E) ,Molecular ion peak,base peak, metastable ions,Nitrogen rule, effect of isotopes, Rules for fragmentation, Mclafferty rearrangement, retro Diels-Alder fragmentation, Problems based on analysis of mass spectra of various organic compounds	
REFERENCES		

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