

**SYLLABUS FOR URET EXAMINATION 2017-18**  
**PG DEPT. OF CHEMISTRY, BERHAMPUR UNIVERSITY**

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**PART -I: RESEARCH METHODOLOGY**

**Unit-I: RESEARCH METHODOLOGY AND DATA ANALYSIS :**

Meaning and Objectives of Research, Methods of Data Collection: Interpretation and Report Writing: , Writing a Research Report, Precautions for Writing Research Reports, Research processes - scientific research, formation of the topic, hypothesis, conceptual definitions, operational definition, gathering of data, analysis of data, revising of hypothesis, Conclusion.

**UNIT 2: RESEARCH PUBLICATIONS:**

Literature survey - Journals, books and reports. Reference, Searching library databases and develop effective search techniques, , bibliographies and the use of Endnote, Use of PowerPoint and how to design an effective oral presentation, informative outlines. Group discussion of a primary research article, writing summaries, peer review. Group presentations of primary research articles. Elements of scientific writing-Abstract and Introduction. Elements of scientific writing-Abstract and Introduction. Elements of scientific writing-Grant proposals Articles: Short Communication, Article, Full articles, Reports, Reviews, Citations, H-10, Index, i-Index, Impact factor, What is ISBN and ISSN number, What is patent, Guide lines of patenting.

**Unit-3: APPLICATIONS OF COMPUTERS IN CHEMISTRY**

History of development of computers, super computer systems. Personal computers. General awareness of computer hardware, CPU, input and output devices, memory, other peripheral devices, auxiliary storage devices. Basic knowledge of computer systems, softwares - System softwares and application softwares Programming languages: machine language, assembly language and high level languages. Interpreter and compiler. Flow charts and Algorithms. General awareness of operating systems: Disk operating system, Windows, Macintosh, Linux. General awareness of Software packages and other scientific application packages. Applications and uses of common softwares in chemistry, Origin, Chems sketch, Chemdraw. Chem draw, Gaussian, Sparton, Mercury, CCDC. Basic ideas on the use of Internet in Chemistry education.

**Unit-4: CHROMATOGRAPHIC & ANALYTICAL TECHNIQUES :**

Basic principles of chromatography, Determining purity of sample. Gas chromatography (GC): Liquid Chromatography (LC) and Principles of high performance Liquid Chromatography (HPLC), Principles of Thin Layer Chromatography (TLC).

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Basic principles of UV-visible, EPR, IR, NMR, XRD, AAS, AES, TG, DTA, DSC, Mossbauer, fluorimetric and phosphorimetric methods. Principles and applications of polarography, amperometry, coulometry and cyclic voltametry.

An integrated problem solving approach to the elucidation of structures of organic and Inorganic compounds based on UV, IR, NMR ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$ ), EPR, XRD, and Mass spectral techniques. Modern NMR experiments: NOE, APT, DEPT, HOMCOR ( $^1\text{H}$ - $^1\text{H}$ ) and HETEROCOSY ( $^1\text{H}$ - $^{13}\text{C}$ ).

## PART -II: CHEMISTRY

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### UNIT 1: ORGANIC CHEMISTRY

Aromaticity, Homo-, hetero-, and non-aromatic compounds, Conformation of cycloalkanes and decalins. Effect of conformation on reactivity. Optical activity of biphenyls, allenes and spirans, Asymmetric synthesis, Noyeri Reduction, Sharpless Epoxidation, Racemic modification, Kinetic and Dynamic Resolution of racemic modification, Absolute and relative configuration, R-S nomenclature, Optical purity, E-Z-notation, Threo- and erythro-, Specific Rotation, HPLC, TLC.

Gilman's reagent, CBS Catalyst, Baker's yeast catalyst, LDA, AIBN, DCC,  $\text{Me}_3\text{SiI}$ ,  $\text{Bu}_3\text{SnH}$ ,  $\text{RCO}_3\text{H}$ ,  $\text{Pb}(\text{OAc})_4$ , PPA, PCC, PDC, Diazomethane, Ozone, Borane-Oxidation, Mercuration-Hydration, Birch Reduction,  $\text{NaBH}_4$ ,  $\text{LiAlH}_4$ , DIBAL, Woodward-prevost hydroxylation, Barton and Shapiro reaction, Hoffmann - Loffler-Freytag; Miyamura, Stille, Negishi and Kamada coupling. Peterson synthesis, Beckmann rearrangement, Electrocyclic reactions: Disrotatory and Conrotatory rotation,  $4n$ ,  $4n+2$  and allylic system, Cycloaddition reaction :  $2+2$  and  $4+2$  cycloaddition, 1,3-Dipolar cycloaddition, Cheletropic reactions, Sigmatropic rearrangements, Claisen Rearrangement, Cope rearrangement, Bayer villager reaction. Barton Reaction, Norrish Type Reaction.

### UNIT 2: INORGANIC CHEMISTRY

VSEPR Theory, Crystal Field Theory, Degenerate orbitals, borazine, phosphorazine and their derivatives, borides and carbides, higher boranes, carboranes, metallaboranes, and metallo-carboranes, compounds with metal-metal multiple bond, Hemoglobin and Myoglobin.

Acid and Base hydrolysis, Factors affecting hydrolysis, Substitution reactions in square planar complexes, Trans effect, Mechanism of one electron reactions, Outer-sphere type reactions, Cross reactions and Marcus-Hush theory, Inner sphere type reactions. Boranes, Synthesis and reactions of cyclopentadienyl metal carbonyls, Ferrocene, cyclopentadienyl metal hydrides,

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Dissociation & Substitution, Oxidative addition & carbonylation, Oxygen transfer from Peroxo and Oxo Species, Reductive & Hydride elimination, Insertion, Displacement and Isomerization reaction, Hydrogenation, Hydrosilation and Hydrocyanation of unsaturated compounds, Hydroformylation, Wacker (Smidt) Process, Olefin Metathesis, Fischer-Tropsch synthesis, Zeigler-Natta polymerization, Water gas reaction.

### UNIT 3: PHYSICAL CHEMISTRY

Collision theory of reaction rate, Activated complex theory, Arrhenius equation, Ionic reaction, Singlet and triplet excitation mechanism, Phase rule, Group, Subgroup and Classes, Symmetry elements and Symmetry operations, Symmetry Point group, Matrix representation of point groups and matrix representation for the  $E$ ,  $C_n$ ,  $\sigma_v$ ,  $S_n$ , Nomenclature and symmetry classification of molecules, Irreducible representation and Orthogonality theorem, Standard reduction, Character table ( $C_{2v}$ ,  $C_{3v}$ ,  $C_{4v}$ ,  $C_{2h}$ ,  $D_2$ ,  $D_{2d}$ ).

Entropy, free energy and laws of thermodynamics, Partial molar properties, Chemical potential, Effect of temperature and pressure, Determination of partial molar properties. Concept of fugacity. Nernst heat theorem and its application. Third law of thermodynamics, Experimental determination of entropy by third law. Maxwell-Boltzmann statistics, Partition function (translational, vibrational, rotational and electronic) for diatomic molecules, relationship between and thermodynamic function (internal energy, enthalpy, entropy and free energy), Calculation of equilibrium constant, Fermi-Dirac statistics, Bose-Einstein statistics, Distribution law and its application to metal.

### UNIT 4: SPECTROSCOPY

Basic Principle and instrumentations of UV, IR, NMR, MASS, EPR and Mossbauer spectroscopy. Combined approach for determination of structure of organic and inorganic compounds. molecules. Wood-ward Hoffmann rule for  $\lambda_{max}$  determination. Chemical shift, Spin-spin interaction, Shielding mechanism, Chemical shift values and correlation to protons bonded to carbon and other nuclei, Chemical exchange, Effect of deuteration, Spin-spin interaction, Shift reagent, NOE, Coupling constant J value, COSY, DEPT, INDEQUATE techniques. Ionization techniques, EI, CI, FD and FAB, Molecular-ion peak, Metastable ions, Mc-Lafferty rearrangement, High resolution mass spectrometry,

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