

## M.Sc. CHEMISTRY SEMESTER I FROM ACADEMIC YEAR 2023-24

### PAPER I - PHYSICAL CHEMISTRY (MAJOR)

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#### Course Outcome

Upon successful completion Learner will be able to:

- CO1:** Define state function, exact and inexact differentials, and explain their significance in thermodynamics.
- CO2:** Analyze the relationship between the coefficient of thermal expansion ( $\alpha$ ) and compressibility coefficient ( $\beta$ ) and their impact on material properties.
- CO3:** Explain the concept of fugacity and its significance in describing the behavior of real gases, including its relation to pressure.
- CO4:** Describe the equilibrium constant for real gases in terms of fugacity and understand how it differs from the ideal gas equation.

#### Module 1: Thermodynamics-I

- 1.1:** State function, Exact and inexact differentials, Cyclic rule, Coefficient of thermal expansion ( $\alpha$ ) and Compressibility Coefficient ( $\beta$ ) and relationship between  $\alpha$  and  $\beta$ , Integrating factor. Maxwell equations, Maxwell thermodynamic square. Enthalpy as a function of Temperature and pressure for ideal and real gases **5L**
- 1.2:** Joule Thomson coefficient, Joule Thomson coefficient in terms of van der Waals constants, inversion temperature, Free Expansion of a gas. Relationship between  $C_p$  and  $C_v$ . Mathematical treatment of Entropy concept, Entropy as state function, Thermodynamic equation of state **5L**
- 1.3:** Entropy changes for a system, surrounding and phase transition, Third law of thermodynamics, Evaluation of absolute entropies, determination of absolute entropies in terms of heat capacity data, standard molar entropies and their **5L**

dependence on molecular mass and molecular structure. Residual entropy

## Module 2: Thermodynamics-II

- 2.1:** Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Equilibrium constant for real gases in terms of fugacity. Activity, dependence of activity on temperature and pressure. **5L**
- 2.2:** Thermodynamic functions of mixing: Gibbs energy of mixing, entropy and enthalpy of mixing. Excess functions of non-ideal solutions: excess thermodynamic functions of chemical potential, Gibb's free energy, entropy, enthalpy and volume **6L**
- 2.3:** Partial molar quantities: calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation **4L**

### References:

1. R. P. Rastogi & R. R. Mishra, An Introduction to Chemical Thermodynamics, 6<sup>th</sup> Revised Edition., Vikas Publishing House PVT Ltd.
2. Donald A. McQuarrie and John D. Simon, Physical Chemistry-A Molecular Approach, Viva Books PVT Ltd.
3. Peter Atkins and Julio de Paula, Physical Chemistry, 10<sup>th</sup> Edition, Oxford University Press, Thomson Press (India) Ltd.
4. K. L. Kapoor, A Text Book of Physical Chemistry-Thermodynamics and Chemical equilibrium, 4<sup>th</sup> Edn., Vol.2, Macmillan Publishers India Ltd
5. J. Gareth Morris, A Biologist's Physical Chemistry, 2<sup>nd</sup> edition, ELBS & Edward Arnold Pub. Ltd.

## **PRACTICAL PAPER I - PHYSICAL CHEMISTRY (MAJOR): ANY 8**

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### **Instrumental Experiments**

1. To determine the formula of silver ammonia complex or copper-ethylene diamine complex by potentiometric method.
2. Determination of Hamett constant of m and p amino / nitro benzoic acid by pH measurement.
3. Verification of Ostwald's dilution law and determination of the dissociation constant of a weak monobasic acid conductometrically.
4. Estimate conductometrically the concentration of  $\text{NH}_4\text{Cl}$  salt with NaOH solution.
5. To determine the ionization constant of bromophenol blue.

### Non instrumental Experiments

1. To study the three component system: Water - Acetic acid - Chloroform
2. Determination of heat of solution of benzoic acid / Salicylic acid by solubility measurements.
3. To study the variation in the solubility of  $\text{Ca}(\text{OH})_2$  in presence of NaOH and hence to determine the solubility product of  $\text{Ca}(\text{OH})_2$  at room temperature.
4. To determine the chain linkage in polyvinyl alcohol from viscosity measurement.
5. To determine the equilibrium constant for the reaction:  $\text{CaSO}_4(\text{s}) + 2\text{Ag}^+(\text{aq}) = \text{Ag}_2\text{SO}_4(\text{s}) + \text{Ca}^{2+}(\text{aq})$

### References:

1. Advanced Practical Physical Chemistry, J.B. Yadav, Krishna Publisher Media, Experimental Physical Chemistry, V. D Athawale. P. Mathur, New Age International, 2001.

## PAPER II - INORGANIC CHEMISTRY (MAJOR)

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### Course Outcome

Upon successful completion Learner will be able to:

- CO1:** Identify and describe the reactivity of transition metal complexes, distinguishing between inert and labile complexes.

- CO2:** Explain the mechanisms and factors influencing ligand substitution reactions in different types of complexes.
- CO3:** Analyze the principles and theories underlying electron transfer reactions, such as electron and atom transfer mechanisms, inner and outer sphere mechanisms, and Marcus theory.
- CO4:** Evaluate the synthesis, properties, structure, and bonding of various organometallic compounds

### **Module 1: Inorganic Reaction Mechanisms**

- 1.1:** Introduction, Reactivity of transition metal complexes: Inert and labile complexes,  $SN^1$  and  $SN^2$  reaction mechanism, Types of intermediate/activated complex formed during  $SN^1$  and  $SN^2$  mechanism, Rate of reactions. **3L**
- 1.2:** Mechanism and factors affecting ligand substitution reactions of: (a) Octahedral complexes without breaking of metal-ligand bond (b) Square planar complexes – trans-effect, its theories and applications & (c) Tetrahedral complexes **6L**
- 1.3:** Redox reactions: Mechanism of electron transfer reactions - (a) Electron and atom transfer reactions (b) Inner and outer sphere mechanisms (c) Marcus theory (Numerical expected) & (d) Complementary and non-complementary reactions. **4L**
- 1.4:** Isomerization and racemization reactions **2L**

### **Module 2: Organometallic Chemistry**

- 2.1:** Organometallic compounds of transition metals: Synthesis, properties, Structure and bonding of the following organometallic compounds: (a) Alkyl and Aryl derivatives (b) Carbenes and Carbynes (Fischer and Tropsch) (c) Alkyne complexes [diphenylacetylene platinum (0)] (d) Arene complexes - sandwich [dibenzene chromium (0)] and half sandwich ( $CpMn(CO)_3$ ,  $CpNi(NO)$ ) **8L**
- 2.2:** Organometallics as Catalysts in Organic Reaction, 16 and 18 electron rule: (a) Hydrogenation (b) Asymmetric hydrogenation (c) hydroamination (d) Monsanto process (e) hydroformylation **5L**

**2.3:** Organometallics in medicine, agriculture, and their biological and environmental aspects. **2L**

**References:**

1. D. Banerjee, Coordination Chemistry, Tata McGraw Hill, Delhi, 1993.
2. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions 2nd ed., Wiley, New York, 1967.
3. D. Benson, Mechanisms of Inorganic Reactions in solution, McGraw – Hill, New York, 1968.
4. J. O. Edwards, Inorganic Reaction Mechanisms, Benjamin, New York, 1974.
5. Geeta Tewari, Inorganic Chemistry II, S. Chand Publications, 2018.
6. R. C. Mehrotra and A. Singh, Organometallic Chemistry-A Unified Approach, 2nd ed., New Age International Pvt. Ltd., 2000.
7. Gary O. Spessard and Gary L. Miessler, Organometallic Chemistry, PrenticeHall, 1977.
8. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 5th ed., Wiley Interscience, 2009.
9. K. F. Purcell and J. C. Klotz, Inorganic Chemistry, Saunders, Hongkong, 1977.
10. B. Douglas, D. H. McDaniel and J. J. Alexander. Concepts and Models of Inorganic Chemistry, 2nd Ed., John Wiley & Sons, 1983.
11. James Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4th Edition, Harper Collins, 2006
12. Gopalan and Ramalingam, Concise coordination chemistry 2012.
13. Gary Miessler and Donald Tarr, Inorganic Chemistry, 3rd Ed. Pearson Education, 2004

**PRACTICAL PAPER II - INORGANIC CHEMISTRY (MAJOR): ANY 8**

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### **Instrumental methods of analysis:**

1. Conductometry:
  1. Estimation of chloride in NaCl/KCl using silver nitrate.
  2. Estimation of Boric acid using ammonium hydroxide.
2. Potentiometry:
  1. Estimation of  $\text{Cu}^{2+}$  using sodium thiosulphate.
  2. Estimation of  $\text{Fe}^{2+}$  using ceric ammonium sulphate.
3. Estimation of Ti and V using hydrogen peroxide
4. Spectrophotometer titration of  $\text{Cu}^{2+}$  against EDTA
5. Determination of formation constant by Job's variation method for  $\text{Fe}^{3+}$ -  $\text{SCN}^-$  system.

## **PAPER III - ORGANIC CHEMISTRY (MAJOR)**

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### **Course Outcome**

Upon successful completion Learner will be able to:

- CO1: Apply the principles of axial and planar chirality and utilize configurational descriptors (R, S) to analyze stereochemical features in compounds.
- CO2: Understand and apply the concepts of Prochirality, homotopic, heterotopic, and diastereotopic ligands and faces.

- CO3: Elaborate the mechanism and applications of specific reagents for oxidation-reduction in organic synthesis.
- CO4: Design the synthesis of organic compounds using specific reagents for oxidation reduction reactions.

### **Module 1: Stereochemistry-I**

- 1.1:** Symmetry operations: Rotation, reflection, inversion, rotation- reflection. **4L**  
Identification of the different axes and planes of symmetry.

Molecules with tri and tetra coordinate chiral centres: Compounds with carbon, silicon, nitrogen, phosphorous and Sulphur chiral centres and their relative configurational stabilities

- 1.2:** Molecules with two or more chiral centres: Configurational nomenclature. **3L**  
Constitutionally unsymmetrical molecules: Erythro-threo and syn-anti systems.  
Constitutionally symmetrical molecules with odd and even number of chiral centres: enantiomeric and meso forms, concept of stereogenic, chirotopic and pseudo asymmetric centres.

- 1.3:** Axial and planar chirality: Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R, S) for the following classes of compounds: Allenes, Alkylidene cycloalkanes, Spiranes, Biaryls (including BINOLs and BINAPs), Ansa compounds and Cyclophanes. **4L**

- 1.4:** Prochirality: Homotopic, heterotopic and diastereotopic ligands and faces. **4L**  
Identification using substitution and symmetry criteria.  
Nomenclature of stereo heterotopic ligands and faces. Symbols for stereo heterotopic ligands in molecules with one or more prochiral centres, pro-pseudo asymmetric centre, chiral and prochiral centre; prochiral axis and prochiral plane. Symbols for enantiotopic and diastereotopic faces.

### **Module 2: Oxidation - Reduction**

- 2.1:** Oxidation: General mechanism, selectivity, stereochemistry and important **8L**

applications of the following:

(a) Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt/Pd/Ni) and organic reagents (Chloranil, DDQ).

(b) Dehydrogenation/oxidation of alcohols to aldehydes and ketones: chromium reagents such as  $K_2Cr_2O_7/H_2SO_4$  (Jones reagent),  $CrO_3$ -pyridine (Collin's reagent), PCC (Corey's reagent) and PDC, hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation) and Oppenauer oxidation.

(c) Oxidation involving C-C bonds cleavage: Glycols using  $HIO_4$ ; cycloalkanones using  $CrO_3$ ; carbon-carbon double bond using ozone,  $KMnO_4$ ,  $CrO_3$ ,  $NaIO_4$  and  $OsO_4$ ; aromatic rings using  $RuO_4$  and  $NaIO_4$

(d) Oxidation involving replacement of hydrogen by oxygen: Oxidation of allylic  $CH_2$  to CO by  $SeO_2$ , Oxidation of aryl methane by  $CrO_2Cl_2$  (Etard oxidation).

7L

**2.2: Reduction:** General mechanism, selectivity, stereochemistry and important applications of the following reducing:

(a) Reduction of CO to  $CH_2$  in aldehydes and ketones –Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification. Ra-Ni desulfurization of Thioketal (Mozingo reduction)

(b) Metal hydride reduction: Boron reagents ( $NaBH_4$ ,  $NaCNBH_3$ ,  $Na(OAc)_3BH$ , Aluminium reagents ( $LiAlH_4$ , DIBAL-H, Red Al, L and K selectrides), MPV reduction,  $NH_2NH_2$  (diimide reduction)

(c) Dissolving metal reductions: using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid  $NH_3$  mediated reduction (Birch reduction) of aromatic compounds and acetylenes.



### References:

1. D, Nasipuri, Stereochemistry of Carbon Compounds: Principles and Applications, 3rd Edition, New Age International Ltd.
2. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India.
3. P. S. Kalsi, Stereochemistry, 4<sup>th</sup> edition, New Age International Ltd.
4. M. J. T. Robinson, Organic Stereochemistry, Oxford University Press, New Delhi, India edition, 2005.
5. Jonathan Clayden, Nick Greeves and Stuart Warren Organic Chemistry (2nd Edition).
6. Seyan Ege, Organic Chemistry: Structure and Reactivity, 5th Edition.
7. Ratan Kumar Kar, Redox and Reagents in Organic Chemistry by (Volume 1) NCBA Publication.
8. S.N Sanyal, Reactions, Rearrangements and Reagents.
9. Michael H Nantz, W. W. Freeman and Company, Modern Organic Synthesis ,1st Edition.

## **PRACTICAL PAPER III - ORGANIC CHEMISTRY (MAJOR)**

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### **Chemical separation of binary mixtures:**

1. Solid-Solid mixture (including water soluble component) (4)
2. Solid-liquid mixtures (4)

### References:

1. I. Vogel, Practical Organic Chemistry, 5th edition.
2. H. Middleton, Systematic Qualitative Organic Analysis.

## **PAPER IV - ANALYTICAL CHEMISTRY (MAJOR)**

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### **Course Outcome**

Upon successful completion Learner will be able to:

- CO1:** Classify and describe analytical methods and instruments used in chemical analysis.
- CO2:** Explain sensitivity, detection limit, and dynamic range in analytical measurements.
- CO3:** Explain the principles and applications of IR and UV-Visible spectroscopy techniques.
- CO4:** Discuss the instrumentation of IR and UV-Visible spectroscopy techniques

## **Module 1: Introduction to Analytical Chemistry and Quality**

- 1.1: Recapitulation:** Classification of Analytical methods, An overview of analytical methods, Types of instrumental methods **4L**  
Instruments for analysis, data domains, electric and non-electric domains, detectors, transducers, sensors, sensitivity, detection limit and dynamic range.
- 1.2: Performance criteria of the method:** calibration curve, standard addition and internal standard methods. selection of analytical method, performance characteristics of instruments, figures of merit **6L**
- 1.3: Quality in analytical chemistry:** quality systems in chemical laboratories, cost and benefits of a quality system, types of quality standards for laboratories **5L**  
Total quality management, quality audits and quality reviews, responsibility of laboratory staff for quality

## **Module 2: Spectroscopic Technique I**

- 2.1: IR Spectroscopy:** Introduction, basic principle, types of molecular vibrations, vibrational modes, vibrational coupling and applications of IR regions. **7L**  
**Dispersive and non-dispersive IR:** Instrumentation in detail, working and its application, FT-IR: Principle instrumentation and working, Qualitative and quantitative application. (Numerical is expected).
- 2.2: UV-Visible Absorption Spectroscopy:** Introduction, basic principle, absorbing species, Auxochrome and chromophore, Aromatic systems, solvent effect. **8L**  
**Application of UV-VIS spectroscopy:** Derivative, Simultaneous and dual wavelength spectrometry: principle, instrumentation and working, application (Numerical is expected)

## **References:**

1. Introduction to instrumental analysis, R. D. Braun, McGraw Hill (1987)
2. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A.

Settle Jr 7th Ed CBS (1986)

3. Fundamentals of Analytical Chemistry, D.A. Skoog and D. M. West and F. J. Holler Holt- Saunders 6th Edition (1992)
4. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th Edition (1998)
5. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N. Y 1997
6. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986)

## **PRACTICAL P IV - ANALYTICAL CHEMISTRY (MAJOR): ANY 8**

1. Determination of amount of Cr (III) and Fe (III) individually in a mixture of two by Complexometric titration
2. Solvent Extraction: (1) Fe (III) & Mg (II) **OR** (2) Fe (III) & Ni (II)
3. Water analysis: Hardness, alkalinity, salinity, acidity
4. Anion exchange chromatography: (1) Ni (II) & Zn (II) **OR** (2) Co(II) & Ni(II)
5. Determination of Iodine value and Acid value of given oil sample
6. TLC and Column chromatography: separation of a mixture of ortho and para nitro-anilines.
7. Assay of Chlorambutol using precipitation titration
8. To carry out assay of the sodium chloride injection by Volhard's method **OR** To carry out assay of a given sample of saline by Mohr's method.

9. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin
10. To determine the number of nitro groups in the given compound using  $\text{TiCl}_3$ .

### References

1. Inorganic quantitative analysis by Vogel sixth edition.
2. Pharmacopoeia of India
3. Biochemical methods, Sadashivam and Manichem, New age international publication
4. General Chemistry experiments by Elias, Universities Press

## PAPER V - DISCIPLINE SPECIFIC ELECTIVE 01

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### Course Outcome

Upon successful completion Learner will be able to:

- CO1:** Explore the role of metal ions in biological systems and their detoxification.
- CO2:** Understand different compound structures ( $\text{AB}$ ,  $\text{AB}_2$ ,  $\text{AB}_3$ ,  $\text{A}_2\text{B}_3$ ,  $\text{ABO}_3$ ,  $\text{AB}_2\text{O}_4$ ).
- CO3:** Understand instruments and components used in HPLC and GC, including mobile phase reservoirs, pumping systems, sample injection, LC columns, and detectors.
- CO4:** Understand different thermoanalytical methods.

### Module 1: Bioinorganic and Solid State Chemistry

#### 1.1: Bioinorganic Chemistry

7L

Introduction, Role of metal ions in biological systems. Toxic metal ions and



their detoxification, chelation therapy/chelating agents in medicine. Recent advances in cancer chemotherapy using chelates. Iron in Ferritin, Transferrin, Fe-S clusters, Porphyrin based systems.

**1.2: Solid State Chemistry**

**8L**

Structures of Compounds of the type:

(a) AB [PbO and CuO]

(b) AB<sub>2</sub> type [ $\beta$ -cristobalite, CaC<sub>2</sub> and Cs<sub>2</sub>O]

(c) AB<sub>3</sub> (ReO<sub>3</sub>, Li<sub>3</sub>N), A<sub>2</sub>B<sub>3</sub> type (Cr<sub>2</sub>O<sub>3</sub> and Bi<sub>2</sub>O<sub>3</sub>), ABO<sub>3</sub> relation between ReO<sub>3</sub> and perovskite BaTiO<sub>3</sub> and its polymorphic forms, AB<sub>2</sub>O<sub>4</sub> type, normal, inverse, and random spinel structures.

**Module 2: Separation and Thermoanalytical Techniques**

**2.1: HPLC & GC Technique**

**8L**

Instruments for HPLC: Mobile phase reservoirs and solvent treatment system, pumping systems, sample injection systems, LC Columns, types of column packing, detectors: Absorbance detector, Refractive Index detector, column efficiency in LC, applications.

Instruments for GC: Carrier gas system, sample injection systems, column oven, temperature programming, GC Column, stationary phase, detectors (coulometric, thermionic ionization detectors), applications.

**2.2: Thermoanalytical Techniques**

**7L**

Introduction, Principle, instrumentation and applications of thermal methods –

1. Thermogravimetric analysis
2. Differential Thermal analysis
3. Differential Scanning Calorimetry

## References:

### Bioinorganic Chemistry

1. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.
2. R. W. Hay, Bioinorganic Chemistry, Ellis Harwood, England, 1984.
3. J. A. Cowan, Inorganic Biochemistry-An introduction, VCH Publication, 1993.
4. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Publications, Mill Valley, Californic, 1994.

### Solid State Chemistry

4. A. R. West, Solid State Chemistry and Its Applications, John Wiley & Sons, New York, 1987.
5. L. V. Azaroff, Introduction to solids, Tata McGraw Hill Book Co., New Delhi, 1977.
6. H. V. Keer, Principles of Solid State, Wiley Eastern Ltd., 1993.
7. C. N. R. Rao and G. Gopalkrishnan, New Directions in solid state chemistry, 2nd Ed., Cambridge University Press, (1997).

### HPLC, GC and Thermoanalytical techniques

1. Introduction to instrumental analysis, R. D. Braun, McGraw Hill (1987)
2. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr 7th Ed CBS (1986)
3. Fundamentals of Analytical Chemistry, D.A. Skoog and D. M. West and F. J. Holler Holt- Saunders 6th Edition (1992)

4. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th Edition (1998)
5. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N. Y 1997
6. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986)

## **PAPER V - DISCIPLINE SPECIFIC ELECTIVE 02**

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### **Course Outcome**

Upon successful completion Learner will be able to:

- CO1:** Recall types and synthesis methods of nanomaterials.
- CO2:** Understand properties of nanomaterials and identify important nanomaterials and their applications.
- CO3:** Classify solar cells and understand their key elements.
- CO4:** Explain principles and applications of wind and geothermal energy.

### **Module 1: Chemistry of Nano materials**

- 1.1:** Introduction, types of Nanomaterials 8L  
Synthesis of Nanomaterials: Physical methods, Chemical methods and





biological methods.

Properties of Nano material: Mechanical, structural, electrical, optical and magnetic properties.

**1.2:** Some important Nanomaterials: carbon nanotubes, porous silicon, core shell particles, Au and Ag Nano material. **7L**

Applications of Nanomaterials: Electronic, Medicine, Infrastructure, automobiles, Agriculture, etc.

## **Module 2: Renewable Energy Sources**

**2.1:** Solar Cell - Classification of Solar cells - (1) First generation - Single crystalline, Poly crystalline, (2) Second Generation - Thin film, CdS, CIGs, (3) Third Generation - Polymer based, DSSC, Perovskites, Hybrid, Quantum Dots, Multi Junction Tandem cells. (And/Or) Organic, Inorganic and Hybrid cells. Key elements of Silicon Solar cell, PV Solar cell, Module, panel and array. Solar thermal systems types, applications of Solar PV and Solar Thermal systems. **7L**

**2.2:** Wind Energy: Introduction, Principle of wind energy conversion, Advantages and disadvantages of wind mills, Applications of wind energy. **4L**

**2.3:** Geothermal energy: Introduction, Estimates of Geothermal Power, Nature of geothermal fields, Geothermal resources, Hydrothermal ( convective) Resources, Geo pressured resources **4L**

## **References:**

### **Nano Chemistry**

1. Nano-chemistry; Kenneth J. Klabunde, Gleb B. Sergeev
2. Nanochemistry: A Chemical Approach to Nanomaterials; Geoffrey A Ozin, André Arsenault

3. Nanomaterials and Nanochemistry; C. Bréchnac, P. Houdy, M. Lahmani.

### **Renewable Energy Sources**

4. Solar Energy Principles, Thermal Collection & Storage, S.P.Sukhatme: Tata McGraw Hill Pub., NewDelhi
5. Non-Conventional Energy Sources, G.D.Rai, NewDelhi
6. Renewable Energy, power for a sustainable future, Godfrey Boyle,2004,
7. The Generation of electricity by wind, E. W. Golding.
8. Non-Conventional Energy Resources by B.H. Khan, Tata McGraw Hill Pub.,2009.
9. Fundamentals of Renewable Energy Resources by G.N.Tiwari, M.K.Ghosal, Narosa Pub., 2007
10. Non-Conventional Energy Resources by B.H. Khan, Tata McGraw Hill Pub., 2009. (Ch:6)
11. Non-Conventional Energy Resources by Shobh Nath Singh, Pearson India., 2016. (Ch:2, 4)
12. Solar Cells: From Materials to Device Technology edited by S. K. Sharma, Khuram Ali, Springer (2020)
13. Rational Design of Solar Cells for Efficient Solar Energy Conversion edited by Alagarsamy Pandikumar, Ramasamy Ramaraj, Wiley (2018).
14. Energy fables, Edited by edited by Jenny Rinkinen, Elizabeth Shove, Jacopo Torriti, Routledge a T&F group, (2019)

## **PRACTICAL PAPER V - DISCIPLINE SPECIFIC ELECTIVE 01/02**

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### **(ANY 8)**

#### **Solid state Chemistry**

1. Limestone Ore: Loss on ignition, Ca by EDTA method
2. Solder Alloy: Sn content by gravimetrically as oxide, Pb content by complexometric method.

#### **Bioinorganic Chemistry**

1. Estimation of calcium in milk/food sample by EDTA titration.
2. Estimation of iron from iron tablet by colorimetry.

#### **HPLC & GC**

1. To determine efficiency of the given column by using HPLC.
2. To separate three alcohols and determine purity of ethanol from given mixture using GC.

#### **Thermoanalytical Techniques**

### Theoretical interpretation

1. Thermal degradation profile of common polymers (PVC, PMMA, PTFA, PI)
2. Kinetics of decomposition of sodium bicarbonate; a differential scanning calorimetry experiment
3. Analysis of the Thermal Properties of Ammonium Nitrate and Polystyrene by Differential Scanning Calorimetry (DSC).

### Chemistry of Nanomaterials

1. Biosynthesis of SnO<sub>2</sub> nanoparticles/Ag nanoparticles and characterization by UV-vis spectrophotometer.
2. To determine UV-vis characteristics of chemically synthesized CdS, ZnO, ZnS, Ag and SnO<sub>2</sub> nanoparticles.

### References:

1. Advanced Practical Physical Chemistry, J.B. Yadav, Krishna Publisher Media, ISBN - 9788182830967
2. Experimental Physical Chemistry, V. D Athawale. P. Mathur, New Age International, 2001. ISBN - 81-224-1336-6
3. A. I. Vogel, Quantitative Inorganic Analysis
4. J. D. Woolins, Inorganic Experiments
5. Palmer, Inorganic Preparations
6. G. Raj, Advanced Practical Inorganic Chemistry
7. P. C. Kamboj, University Practical Chemistry
8. I. Vogel, Practical Organic Chemistry, 5<sup>th</sup> edition.
9. H. Middleton, Systematic Qualitative Organic Analysis

## M.Sc. CHEMISTRY SEMESTER II FROM ACADEMIC YEAR 2023-24

### PAPER I - PHYSICAL CHEMISTRY (MAJOR)

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#### Course Outcome

Upon successful completion Learner will be able to:

- CO1:** Recall methods for determining rate laws.
- CO2:** Explain the application of steady state approximation.
- CO3:** Study of fundamental postulates of Quantum Chemistry
- CO4:** Apply principles of quantum mechanics to free particles and particle in a box systems.

#### Module 1: Chemical Kinetics

- 1.1:** Methods of determining rate laws, Steady state approximation and its **4L** applications, Mechanism of photochemical (hydrogen-bromine and hydrogen-chlorine), chain reaction (hydrogen-bromine reaction) consecutive reactions.



- Inorganic mechanisms: Formation and decomposition of phosgene, decomposition of ozone.
- 1.2:** Organic Decompositions: pyrolysis of acetaldehyde, Decomposition of ethane, Decomposition of acetaldehyde. **3L**
- 1.3:** Gas phase reactions: Reaction between  $H_2$  and  $O_2$ , Semenov-Hinshelwood-Thompson Mechanism. Explosion Limits and factors affecting explosion limits. **2L**
- 1.4:** Activated complex theory, thermodynamic interpretation, comparison of Eyring and Arrhenius equations. **3L**
- 1.5:** Elementary Reactions in Solution: Solvent Effects on reaction rates, Reaction between ions- influence of solvent dielectric constant, influence of ionic strength, **3L**

## **Module 2: Quantum Chemistry**

- 2.1:** Postulates of Quantum Mechanics Time independent Schrödinger wave equation. **2L**
- 2.2:** Application of quantum mechanics to the following systems: **6L**
- a) Free particle, wave function and energy of a free particle.
  - b) Particle in a one, two and three-dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels.
  - c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.
- 2.3:** Rigid rotor, spherical coordinates Schrodinger wave equation in spherical coordinates, separation of the variables, the phi equation, the theta equation, wave function, quantization of rotational energy, spherical harmonics. Space quantization of angular momentum. **7L**

### References:

1. R. P. Rastogi & R. R. Mishra, An Introduction to Chemical Thermodynamics, 6<sup>th</sup> Revised Edition., Vikas Publishing House PVT Ltd.
2. Donald A. McQuarrie and John D. Simon, Physical Chemistry-A Molecular Approach, Viva Books PVT Ltd.
3. Peter Atkins and Julio de Paula, Physical Chemistry, 10<sup>th</sup> Edition, Oxford University Press, Thomson Press (India) Ltd.
4. K. L. Kapoor, A Text Book of Physical Chemistry-Thermodynamics and Chemical equilibrium, 4<sup>th</sup> Edn., Vol.2, Macmillan Publishers India Ltd
5. J. Gareth Morris, A Biologist's Physical Chemistry, 2<sup>nd</sup> edition, ELBS & Edward Arnold Pub. Ltd.
6. Quantum Chemistry - Levine
7. Handbook of Molecular Physics and Quantum Chemistry - Ermuhammad B. Dushanov Mirzoaziz A. Khusenov
8. Elementary Quantum Chemistry - Frank L. Pilar
9. Introduction to quantum chemistry - Carole R Gatz
10. Quantum Theory for Chemical Applications - Jochen Autschbach
11. Principles and Applications of Quantum Chemistry - V.P. Gupta

12. Physical Chemistry, Volume 2 - Peter Atkins, Julio de Paula

## **PRACTICAL PAPER I - PHYSICAL CHEMISTRY (MAJOR): ANY 8**

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### **Instrumental Experiments**

1. Study the effect of substituents on the dissociation constant of acetic acid by conductometrically.
2. Determination of pK<sub>a</sub> values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrodes.
3. Kinetic study of ethyl acetate by conductometric method.
4. Titration of a mixture of Trichloroacetic acid, Monochloroacetic acid and Acetic acid with sodium hydroxide conductometrically.
5. To determine the rate constant and the order of the reaction for the alkaline hydrolysis of crystal violet



6. To determine the rate constant and the order of the reaction between persulphate and iodide ions by colorimetry.
7. To determine the molar conductance of a weak electrolyte at infinite dilution hence to determine its dissociation constant.
8. To determine hydrolysis constant and degree of hydrolysis of ammonium chloride and hence to estimate the dissociation constant of the base.

### **Non instrumental Experiments**

1. To study the influence of ionic strength on the reaction between  $K_2S_2O_8$  and KI.
2. Investigation of the reaction between acetone and iodine.

### **References:**

1. Advanced Practical Physical Chemistry, J.B. Yadav, Krishna Publisher Media,
2. Experimental Physical Chemistry, V. D Athawale. P. Mathur, New Age International, 2001.

## **PAPER II - INORGANIC CHEMISTRY (MAJOR)**

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### **Course Outcome**

Upon successful completion Learner will be able to:

- CO1:** Learn matrix representation of symmetry operations and distinguish between reducible and irreducible representations.
- CO2:** Analyze the symmetry properties of molecules, considering optical activity and dipole moment restrictions.
- CO3:** Classify inorganic ring, cage and cluster compounds on the basis of their structural type
- CO4:** Explore the reactivity, structures and bonding of silicates, boranes, and phosphazenes.

### **Module 1: Molecular Symmetry and Group theory**



- 1.1:** Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups. **3L**
- 1.2:** Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules. **2L**
- 1.3:** Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem. Construction of character tables for point groups  $C_{2v}$ ,  $C_{3v}$  and  $D_{2h}$ , structure of character tables, Mulliken's notations for irreducible representations. **5L**
- 1.4:** Reduction formula, application of reduction formula to vibrational modes of water and ammonia molecules. **3L**
- 1.5:** Group, subgroup relationships, descent and ascent in symmetry, correlation diagrams showing relationship between different groups **2L**

## **Module 2: Inorganic Rings, Cages and Metal Cluster Compounds**

- 2.1:** Silicates: Classification and structure **2L**
- 2.2:** Bonding in boranes, Wade's rule, STYX number, Heteroboranes Carboranes, Metal-Metal bonding and Metal Clusters, Zintl ions, Electron Count and Structures of Clusters. **7L**
- 2.3:** Isolobal Analogy and Structures **2L**
- 2.4:** Aluminosilicates, Zeolites: Synthesis, characterization, determination of surface acidity, shape selectivity and applications. **2L**
- 2.5:** Phosphazenes: Preparation ( $N_3P_3Cl_6$  and  $N_4P_4Cl_8$ ), properties and uses. **2L**

### References:

1. F. A. Cotton, Chemical Applications of Group Theory, 2<sup>nd</sup> Edition, Wiley Eastern Ltd., 1989.
2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1966.
3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
4. K.V. Reddy, Symmetry and Spectroscopy of Molecules, 2<sup>nd</sup> Ed., New Age International Publishers, New Delhi, 2009.
5. R. Ameta, Symmetry and Group Theory in Chemistry, New Age International Publishers. 2012.
6. Gurudeep Raj, Advanced Inorganic Chemistry, Vol- II, Krishna Prakashan Media Pvt.Ltd.
7. James Huheey, F. A. Keiter and R.L. Keiter, Inorganic Chemistry – Principles of Structure and Reactivity, 4<sup>th</sup> Edition, Harper Collins, 2006
8. Puri, Sharma and Kalia, Principles of Inorganic Chemistry – 31<sup>st</sup> Edition, Milestone Publishers, 2010.
9. S. Pimpalpure, Rashmi Jain, UshaSoni and S.D. Dwivedi, Advanced Inorganic Chemistry, Vol- II, Pragatiprakashan.
10. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3<sup>rd</sup> Edition.
11. Atkin and Shriver, Advanced Inorganic Chemistry, 6<sup>th</sup> Edition.
12. Gary Miessler and Donald Tarr, Inorganic Chemistry, 3<sup>rd</sup> Ed. Pearson Education, 2004.

## PRACTICAL PAPER II - INORGANIC CHEMISTRY (MAJOR)

### Synthesis and characterization of the following inorganic preparations:

1. Potassium trioxalato chromate

2. Bis (ethylenediamine)copper(II) sulphate
3. Tris(thiourea) copper(I) sulphate
4. Chloropentaammincobalt (III) chloride
5. Synthesis of bis(acetylacetonato)dioxomolybdenum(VI),  $[\text{MoO}_2(\text{acac})_2]$  and qualitative estimation of molybdenum.
6. Synthesis of ZnO nanoparticles and study of its UV spectra.
7. Synthesis and Purity of  $[\text{Mn}(\text{acac})_3]$  by TLC.

### References

1. I. Vogel, Quantitative Inorganic Analysis
2. R. C. Maurya, Inorganic Chemistry
3. J. D. Woolins, Inorganic Experiments
4. Palmer, Inorganic Preparations
5. G. Raj, Advanced Practical Inorganic Chemistry

## PAPER III - ORGANIC CHEMISTRY (MAJOR)

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### Course Outcome

Upon successful completion Learner will be able to:

- CO1:** Explore the preparation and applications of organoborane reagents in organic synthesis, including hydroboration reactions and functional group reduction using diborane.
- CO2:** Constructing carbon-carbon bond in organic molecules using organometallics compounds.
- CO3:** Understand the principles and applications of IR, UV-VIS,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy in structure determination
- CO4:** Apply knowledge of spectroscopy to solve various organic problems for structure

elucidation

### **Module 1: Metals / Non-metals in organic synthesis-I**

- 1.1:** Organoboron compounds: Preparation and applications of organoborane reagents e.g. 9-BBN, catechol borane, Thexylborane, ICPBH<sub>2</sub>, IPC<sub>2</sub>BH in organic synthesis. Hydroboration-mechanism, stereo and regioselectivity. Synthesis of EE, EZ, ZZ dienes and alkynes. Alkylboranes synthesis, mechanism and uses. Functional group reduction by diborane. **5L**
- 1.2:** Organosilicon compounds: Important features of silicon governing the reactivity of C-Si compounds: preparation and important bond forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allylsilanes.  $\beta$ -silylations as intermediate, Peterson olefination. **4L**
- 1.3:** Silyl enol ethers as enolate precursors, iodotrimethylsilane in organic synthesis. **2L**
- 1.4:** Organomagnesium, Organolithium and Organo-copper compounds: Preparation and application. **4L**

### **Module 2: Organic Spectroscopy-I**

- 2.1:** Ultraviolet spectroscopy: Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, solvent polarity. Calculation of absorption maxima by Woodward-Fieser Rules (using Woodward-Fieser tables for values for substituents) for the following classes of organic compounds: conjugated polyenes (cyclic and acyclic), enones and substituted benzene derivatives. **5L**
- 2.2:** Infrared spectroscopy: Fundamental, overtone and combination bands, vibrational coupling, important group frequencies for the common functional groups, factors affecting vibrational frequencies. Principle and applications of FT-IR. **3L**
- 2.3:** NMR spectroscopy: (a) Proton magnetic resonance spectroscopy: Chemical shift, Factors affecting chemical shift, Chemical and magnetic equivalence, **5L**

### Spin-spin

coupling, coupling constant J, Factors affecting J, First order spectra, Geminal and vicinal coupling (allylic and aromatic)

(b) <sup>13</sup>C-NMR spectroscopy introduction: <sup>13</sup>C chemical shifts, calculation of <sup>13</sup>C-chemical shift and examples.

**2.4:** Structure determination involving individual or combined use of the above **2L** spectral techniques.

### References:

1. Carruthers and Iain Coldham, Modern method of organic synthesis. (Cambridge)William, 4th edition.
2. F. A. Caray and R. J. Sundberg, Advance Organic Chemistry Part-B-Plenum Press.
3. R.O.C Norman and J.M. Coxon, Principles of organic synthesis. (Nelsons Thoran), 3rd edition.
4. V. K. Ahluwalia, Rakesh Kumar Parashar, Organic reaction mechanism. 4th edition.
5. P. S. Kalsi, Organic reaction structure and mechanism, 4th edition.
6. Clayden, Greeves, Warren and Wothers, Organic Chemistry, (Oxford).
7. C. Eabon, Organosilicon Compound.
8. H. C. Brown, Organic Synthesis via Boranes.
9. T. P. Onak, Organoborane Chemistry.
10. W. Gerrard, Organic Chemistry of Boron.
11. Donald L. Pavia and Gary M. Lampman, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry.
12. Silversteine and Bassler, Spectrometric Identification of Organic Compounds.
13. P. S. Kalsi, Spectroscopy of Organic compounds.
14. J. Bellamy, Infrared spectra of Complex molecules.
15. I Fleming, Organic Spectroscopy.

## **PRACTICAL PAPER III - ORGANIC CHEMISTRY (MAJOR)**

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### **Organic Preparations**

1. Benzoin to Benzil
2. Bromobenzene to p-nitrobromobenzene
3. Anthracene to Anthracene-Maleic anhydride adduct
4. 5,5-Diphenylhydantoin from urea and benzyl
5. 4-Benzylidene -2-Phenyl oxazol-5-one from hippuric acid and acetic anhydride
6. Anthracene to Anthraquinone
7. Resorcinol to 7-hydroxy-4-methyl coumarin
8. 2-naphthol to 1,1'-Bis-2-naphthol

### **References:**

1. I. Vogel, Practical Organic Chemistry, 5th edition.
2. H. Middleton, Systematic Qualitative Organic Analysis.

## **PAPER IV - ANALYTICAL CHEMISTRY (MAJOR)**

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### **Course Outcome**

Upon successful completion Learner will be able to:

- CO1:** Acquire proficiency in using chromatography methods like partition chromatography, ion chromatography, and affinity chromatography.
- CO2:** Gain knowledge of solvent extraction method and its applications.
- CO3:** Develop skills in utilizing mass spectrometry for ionization and analysis of compounds, including electron impact, chemical ionization, and electrospray ionization methods.

**CO4:** Learn about the working principles of NMR spectroscopy and its applications in studying chemical shifts, relaxation processes, and chemical exchange phenomena.

### **Module 1: Separation Techniques II**

- 1.1:** Partition chromatography, Ion chromatography, Affinity chromatography, **8L**  
HPTLC, Supercritical chromatography, Supercritical fluid extraction, applications.
- 1.2:** Solvent extraction: Recapitulation, factors affecting the solvent extraction of **7L**  
inorganic species, separation of metal ions as chelates, ion association, solvation with suitable examples, concept of [pH] <sup>1</sup>/<sub>2</sub>.

### **Module 2: Spectroscopic Technique II**

- 2.1:** Mass Spectrometry: Introduction, ion source, electron impact source, chemical **7L**  
ionization source, field ionization source, field desorption sources, MALDI, electrospray ionization  
Mass spectrometer: sample inlet system, mass analysers, magnetic sector analyser, time of flight, quadrupole, ion trap, application in organic and inorganic chemistry (Numerical is expected)
- 2.2:** Nuclear Magnetic Resonance (NMR): Introduction, Classical and Quantum **8L**  
description of NMR, relaxation process, chemical shift, Abscissa scales for NMR spectra, interpretation of first order spectra, effect of chemical exchange on spectra.  
NMR spectrometers: Instrumentation, working, applications of <sup>1</sup>H NMR, <sup>13</sup>C NMR, <sup>31</sup>P NMR, <sup>19</sup>F NMR. (Numerical is expected)

### **References:**

7. Introduction to instrumental analysis, R. D. Braun, McGraw Hill (1987)
8. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A.



Settle Jr 7th Ed CBS (1986)

9. Fundamentals of Analytical Chemistry, D.A. Skoog and D. M. West and F. J. Holler  
Holt- Saunders 6th Edition (1992)
10. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5th  
Edition (1998)
11. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N. Y  
1997
12. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986)

## **PRACTICAL P IV - ANALYTICAL CHEMISTRY (MAJOR): ANY 8**

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1. To determine the amount of HCl and H<sub>2</sub>SO<sub>4</sub> and hence weight percent in a mixture of the two by conductometric titration
2. To determine the amount of Fe(II) and Fe(III) present in the given solution by spectrophotometric method using 1:10 phenanthroline solution/ To Determine Fe (III) in the given solution by colorimetric method.
3. To determine the amount of Cr(VI) and Mn(VII) in the given solution by simultaneous spectrophotometric method
4. To determine the amount of potassium in the given fertilizer sample by flame photometry
5. To determine percentage purity of sodium carbonate in washing soda by pH metrically
6. To determine the amount of Ti(III) and Fe(II) in the given solution by titration with Ce(IV) potentiometrically

7. To determine the percentage purity of sodium benzoate via non-aqueous potentiometric titration.
8. Estimation of dairy whitener by flame photometer for its Na<sup>+</sup> content
9. To determine the amount of iodide, bromide and chloride in the given mixture by potentiometric titration using silver nitrate.
10. To determine percentage purity of sodium carbonate in washing soda pH metrically.

### References

5. Inorganic quantitative analysis by Vogel sixth edition.
6. Pharmacopoeia of India
7. Biochemical methods, Sadashivam and Manichem, New age international publication
8. General Chemistry experiments by Elias, Universities Press

## PAPER V - DISCIPLINE SPECIFIC ELECTIVE 01

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### Course Outcome

Upon successful completion Learner will be able to:

**CO1:** Familiarize with enolates and different reactions based on enolate ion mechanisms.

**CO2:** Explore and examine various organic reactions involving carbonyl chemistry.

**CO3:** Illustrate application of electrochemistry for renewables Energy Sources like batteries and fuel cells

**CO4:** Discuss the kinetics of reactions in solid state and Enzyme catalysed reactions.

### Module 1: Carbonyl chemistry and Name reaction

- 1.1: Enolates:** Structure and stability of enolates. Generation of enolates using **5L** nucleophilic and non-nucleophilic bases. Kinetic and thermodynamic control in

regiochemistry of enolates, Reactions of enolates ions.

- 1.2: Name reactions:** Aldol, Claisen, Claisen-Schmidt condensation, Stobbe condensation, Dieckmann reaction. Perkin reaction, Knoevenagel reaction, Benzoin condensation, Mannich reaction, Shapiro reaction, Michael Reaction, Robinson ring annulation, Haloform reaction, Reformatsky reaction. **10 L**

## **Module 2: Electrochemistry and Kinetics of reactions in solids and Enzyme Kinetics**

- 2.1: Batteries:** Working principle, cell reactions and cell performances of Lithium batteries (Primary and Secondary), Lithium based conducting polymer batteries, Silver- anode primary batteries, High temperature solid state batteries. **8L**

**Fuel cells:** Classification,  $H_2 - O_2$  fuel cell, Alkaline fuel cells, Phosphoric acid fuel cells, Solid polymer electrolyte fuel cells, Solid oxide fuel cells, Biochemical fuel cells.

- 2.2: Kinetics of reactions in solids :** Rate laws for reactions in solid, the parabolic rate law, the first order rate law, the contracting sphere rate law, contracting area rate law, some examples of kinetic studies. **7L**

**Enzyme Kinetics:** Enzyme action, Kinetics of reactions catalysed by enzymes- Michaelis- Menten analysis, Lime weaver –Burk and Eadie analysis-competitive, uncompetitive and noncompetitive Inhibition.

## **References:**

### **Name Reactions and Carbonyl chemistry**

1. W. Carruthers and Iain Coldham, Modern methods of Organic Synthesis, 4 th Edition Cambridge University Press 2004.
2. Jerry March, March's Advanced Organic Chemistry, 6 th edition, 2007, John Wiley and sons.
3. V. K. Ahluwalia, R. K. Parashar, Organic Reaction Mechanism, 4 th edition, Narosa Publication.

4. J. Clayden, S. Warren, N. Greeves, P. Wothers, Organic Chemistry, 1st Edition, Oxford University Press (2001).
5. Gautam Brahmachari, Organic Name reaction: a unified approach, Narosa publication.
6. Name Reactions: A Collection of detailed mechanisms and synthetic applications, Jie Jack Li, Springer-Verlag Berlin Heidelberg.

### **Electrochemistry and Kinetics of reactions in solids**

1. R. Narayan and B. Vishwanathan, Chemical and Electrochemical Energy Systems, Universities Press (India) Ltd. 1998
2. Modern Electrochemistry 1: Ionics, Modern Electrochemistry 2A: Fundamentals of Electrodeics, 2nd Edition by John O'M. Bockris Amulya K.N. Reddy.
3. Principles of instrumental analysis: Skoog, Holler, Niemann, 9th edition
4. March's advanced organic chemistry: reactions, mechanism and structures Michael B Smith and Jerry March 6th Edition.
5. Chemical Kinetics of Solids, Hermann Schmalzried, Wiley VCH

## **PAPER V - DISCIPLINE SPECIFIC ELECTIVE 02**

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### **Course Outcome**

Upon successful completion Learner will be able to:

- CO1:** Understand and apply Linear Free Energy Relationship (LFER) and the Hammett equation. (Knowledge/Application)
- CO2:** Understand the concepts of bioenergetics, including entropy, free energy changes, endergonic and exergonic processes, coupled reactions, and the role of ATP in bioenergetics.
- CO3:** Evaluate the structures, synthesis and applications of macromolecules (crown ether, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins) and molecular receptors.
- CO4:** Understand the basic theory, working principles, and instrumentation of electrophoresis, including factors affecting separation, resolution, and detection systems.

## Module 1: Physico-Organic Chemistry and Bioenergetics

**1.1: Linear free energy relationship (LFER):** Introduction and concept in organic chemistry, Hammett equation - substituent constant ( $\sigma$ ), reaction constants ( $\rho$ ), Limitation, Application, Deviations from Hammett equation. **8L**

The Taft model - Polar substituent constant ( $\sigma^*$ ), Steric substituent constant ( $E_s$ ), Polar Sensitivity Factor ( $\rho^*$ ),

Oka-moto Brown Equation, Yukawa-Tsuno equation

**1.2: Bioenergetics:** Entropy and free energy changes of a biochemical reaction. Endergonic and exergonic processes, coupled reactions, ATP and its role in bioenergetics. **7L**

**Statistical Mechanics in Biopolymers:** Chain Configuration and Conformation of Macromolecules, Statistical distribution end-to-end dimensions, Thermodynamic probability of chain, Calculation of average dimensions for various chain structures. Donnan membrane equilibrium, membrane hydrolysis.

## Module 2: Supramolecular Chemistry and Capillary Electrophoresis

**2.1: Supramolecular Chemistry** **7L**  
Structures, properties and applications of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.

Molecular recognition and catalysis, Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.

**2.2: Capillary Electrophoresis** **8L**  
Introduction to electrophoresis: basic theory, instrumentation, working, detection system, factor affecting separation, resolution and application (GE, CE, CGE, SDS-PAGE).

## References:

### Physico-Organic Chemistry

1. John McMurry, Organic chemistry, 8th edition.
2. Carruthers and Iain Coldham, Modern methods of Organic Synthesis, 4th edition W. Cambridge University Press, 2004.
3. Eric V Anslyn, Dennis A. Dougherty, Modern physical chemistry, University science books, 2006.
4. N. S. Isaacs, Physical Organic Chemistry, ELBS/Longman.

### **Biophysical Chemistry**

1. U. N. Dash, A Text book of Biophysical Chemistry, Macmillan India Ltd.
2. Gurtu and Gurtu, Biophysical Chemistry, Pragati Prakashan
3. Avinash Upadhyay, Kakoti Upadhyay, Nirmalendu Nath, Biophysical Chemistry: Principles and Techniques, Himalaya Publishers

### **Supramolecular Chemistry**

1. D. Nasipuri - Stereochemistry of Organic Compounds: Principles and Applications
2. Jonathan W. Stead and Jerry L. Atwood - Supramolecular Chemistry
3. Katsuhiko Ariga, Toyoki Kunitake and Masa kazu Aono - Supramolecular Chemistry - Fundamentals and applications.

### **Capillary Electrophoresis**

1. Capillary Electrophoresis - Methods and Protocols; Philippe Schmitt-Kopplin
2. Capillary Electrophoresis: Theory and Practice; Paul D. Grossman, Joel C. Colburn
3. Capillary Electrophoresis; Dale R. Baker
4. Capillary Electrophoresis; Schmitt-Kopplin Philippe

## **PRACTICAL PAPER V - DISCIPLINE SPECIFIC ELECTIVE 01/02**

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### **Chemical separation of binary mixtures:**

1. Liquid-liquid mixture (3)

**Organic Preparations:**

1. Solvent free synthesis of Chalcone (Green Synthesis)
2. Bromination of acetanilide (Green synthesis)

**Electrochemistry:**

1. Determination of mean ionic activity coefficient of an electrolyte by emf measurements.
2. To determine the CMC of Sodium Lauryl Sulphate from measurement of conductivities at different concentrations.
3. To determine the formula of the zinc ferrocyanide complex by titration of zinc (II) sulphate with potassium ferrocyanide  $K_4[Fe(CN)_6].3H_2O$ .
4. To determine the rate constant and order of the reaction between persulphate and iodide ions by colorimetry.
5. To investigate the autocatalytic reaction between potassium permanganate and oxalic acid.

**References:**

1. Advanced Practical Physical Chemistry, J.B. Yadav, Krishna Publisher Media, ISBN - 9788182830967
2. Experimental Physical Chemistry, V. D Athawale. P. Mathur, New Age International, 2001. ISBN - 81-224-1336-6
3. A. I. Vogel, Quantitative Inorganic Analysis
4. J. D. Woolins, Inorganic Experiments
5. Palmer, Inorganic Preparations
6. G. Raj, Advanced Practical Inorganic Chemistry
7. P. C. Kamboj, University Practical Chemistry
8. I. Vogel, Practical Organic Chemistry, 5<sup>th</sup> edition.
9. H. Middleton, Systematic Qualitative Organic Analysis